



Seminar Proceedings

## AI and ML in Simulation Driven Design

How do these Technologies Add Value?

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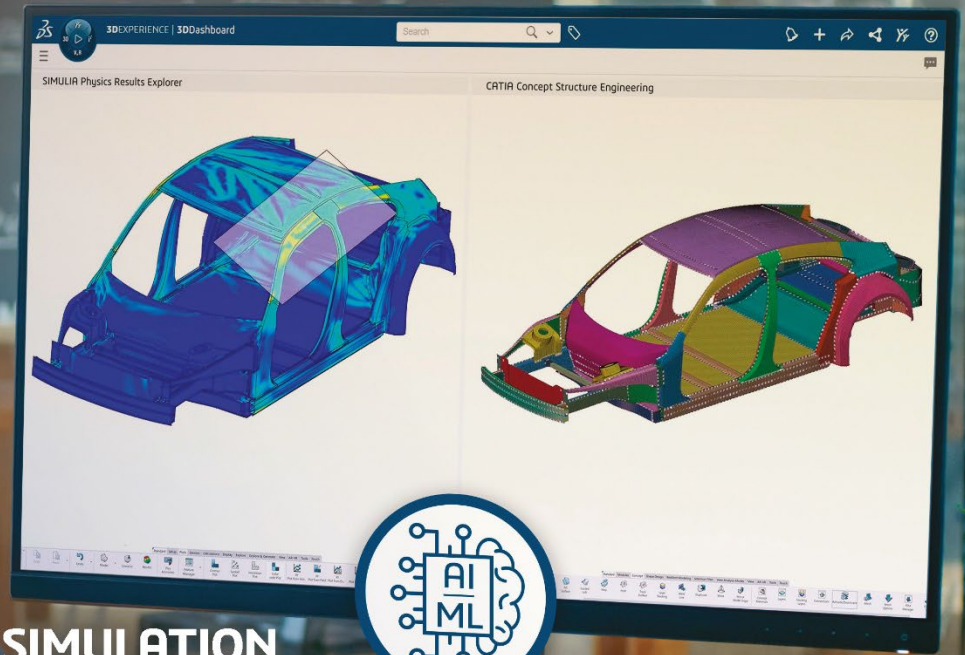
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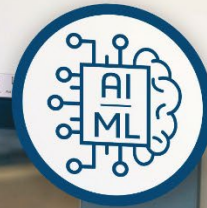
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# **AI-Driven Digital Twins: Bridging the Physical and Digital Worlds in Modern Mecha(tro)nics**

Grzegorz Orzechowski

LUT University

This keynote explores the growing role of AI-driven digital twins in mechanical engineering and mechatronics, highlighting trends like digitalization, electrification, and autonomy. It covers how simulation and modeling support sustainability, cost reduction, and innovation, with real-world examples like automated control of heavy machinery and fatigue monitoring. LUT University's dedication to using these advancements for a brighter, sustainable future will also be emphasized.

# Data-based Design of a Tracking Controller for Planar Closed-loop Mechanisms

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## 1. Summary

Path tracking problems have always been of engineers' interest whether in purely mechanical or mechatronic mechanisms to follow a certain trajectory with desired velocities. Setting up a trajectory controller requires quite some expertise in kinematics and dynamics, especially in case of closed-loop mechanisms. The method introduced in this paper tries to minimize expertise and deep understanding of system kinematics and dynamics by utilizing artificial intelligence (AI) methods as a substitution of such advanced knowledge.

The concept is demonstrated along a first example where a user-defined tracking path is processed by an artificial neural network to define the corresponding geometry of a four-bar linkage (Fig. 1a). In order to realize a desired velocity profile defined by splines, additional neural feedforward networks are trained as models for inverse kinematics and inverse dynamics just from simulation data without any knowledge on the internal structure of the mechanism. Together they provide exact feedback linearization to simplify the control of the torque acting on the crank. To demonstrate general applicability of the proposed control framework, a lambda robot with two degrees of freedom is used as second example, which is also a closed-loop mechanism with the shape of the Greek letter lambda (Fig. 1b).

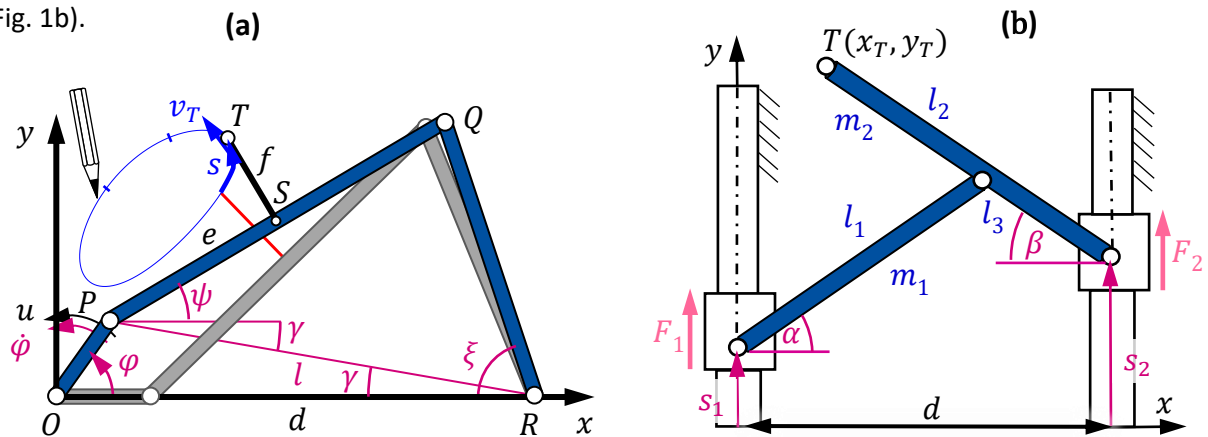


Fig 1. Case studies: Planar four-bar mechanism (a) and lambda robot (b)

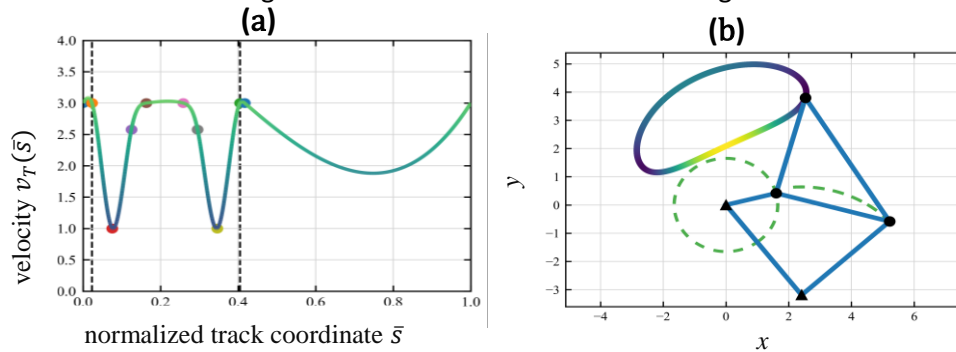
## 2. Four-bar Mechanism Design

Designing a mechanism for a specific task requires deep kinematic expertise. If additionally the velocity shall be prescribed, also dynamic expertise is required. This limits applications due to the high design effort. In the following, a concept for a mechatronic four-bar mechanism will be developed where human expertise is substituted by artificial intelligence.

As a starting point, in Fig. 2a the user defines a desired trajectory as a hand-drawing in the  $(x, y)$ -plane, Fig. 1a, together with speed information how fast the track shall be followed. The latter is defined by setting an arbitrary number of control points, Fig. 2a. If we assume that the user-defined track can be realized by a four-bar mechanism, the first task of a design assistant system is to find associated values for mechanism parameters  $a, b, c, d, e, f$ . Classically this would be done by optimization; here, however, they are predicted by a neural network which was trained by many artificially generated mechanisms [1]. The data for the training set can be generated with classical simulation by randomly assigning



values to the mechanism parameters and computing the corresponding track. For the training set, then only the order of input-output data needs to be reversed. In the specific example, the ANN predicts the mechanism shown in Fig. 2b, with the parameter value provided in the figure caption. The desired velocity profile in Fig. 2a relates the speed  $v_T$  of the tracking point  $T$  to the track coordinate  $s$ , see Fig. 1a. For full information on  $v_T(s)$ , the control points provided by the user are interpolated by splines which is used to design a controller for the moment  $u$  acting on the crank  $\overline{OP}$ .



**Fig 2.** Proposed velocity profile (a) for the hand-drawn trajectory in Fig. 1a resulting in a four-bar linkage (b) with parameter values  $(a, b, c, d, e, f) = (1.652, 3.754, 3.831, 4.001, 0.001, 3.505)$

The control concept to be used is exact feedback linearization requiring an inverse kinematics model  $\dot{\varphi} = \dot{\varphi}(s, v_T(s))$  relating angular crank speed  $\dot{\varphi}$  to the desired velocity profile  $v_T(s) = v_T(s(\varphi))$ , as well as an inverse dynamics model  $u = u(v_T(s))$  relating the crank moment to kinematic quantities. Due to the nonlinearities, a mathematical inversion would be rather tedious, which is why again neural networks are applied. The necessary data is again generated by classical simulation based on randomly chosen initial angular crank velocities  $\dot{\varphi}_0^{(j)}$  resulting in information on crank angle  $\varphi_k^{(j)} = \varphi(t_k; \varphi_0^{(j)})$ , track coordinate  $s_k^{(j)}$  and track speed  $v_{T,k}^{(j)}$ . Corresponding velocities  $\dot{\varphi}_k^{(j)}$  and accelerations  $\ddot{\varphi}_k^{(j)}$  are computed via central time differences [2]. By picking corresponding data from the overall data set

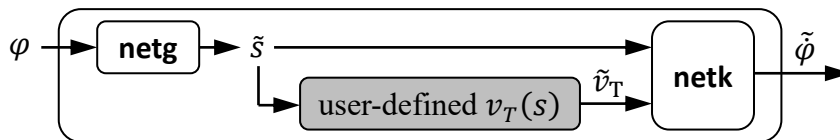
$$\left\{ \left( \varphi_k^{(j)}, \dot{\varphi}_k^{(j)}, \ddot{\varphi}_k^{(j)}, v_{T,k}^{(j)}, s_k^{(j)} \right), k = 0 \dots K, j = 1 \dots J \right\},$$

the required ANNs may be trained.

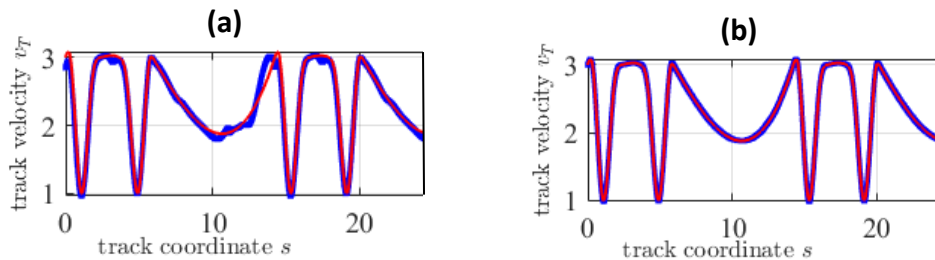
In a first attempt, two ANNs **netg** and **netk** were trained for the inverse kinematics as shown in Fig. 3 to first predict the track length  $s(\varphi)$  and then angular crank velocity  $\dot{\varphi}(s, v_T)$ , respectively:

$$\left( \varphi_k^{(j)}; s_k^{(j)} \right) \xrightarrow{\text{netg}} \tilde{s} \approx s(\varphi), \quad \left( \left( s_k^{(j)}, v_{T,k}^{(j)} \right); \dot{\varphi}_k^{(j)} \right) \xrightarrow{\text{netk}} \tilde{\dot{\varphi}} \approx \dot{\varphi}(s, v_T).$$

However, it turned out that predictions loose exact periodicity, see e.g.  $s \approx 14$  in Fig. 4.



**Fig 3.** Forward control surrogate for relation  $\dot{\varphi}(\varphi)$  integrating the user-defined velocity profile  $v_T(s)$ .



**Fig 4.** Desired velocity (red) track point and predicted values (blue) by a) the network shown in Fig. 3 and b) by **netp** in Fig. 5.

In order to enforce periodicity, Fig. 3 is substituted by a network using periodic inputs  $\sin \varphi$  and  $\cos \varphi$  instead of the crank angle  $\varphi$  itself, see Fig. 5, i.e.,

$$\mathbf{netp}: \left\{ \left( \left( \sin \varphi_k^{(j)}, \cos \varphi_k^{(j)}, v_{T,k}^{(j)} \right); \dot{\varphi}_k^{(j)} \right), k = 0 \dots K, j = 1 \dots J \right\}.$$

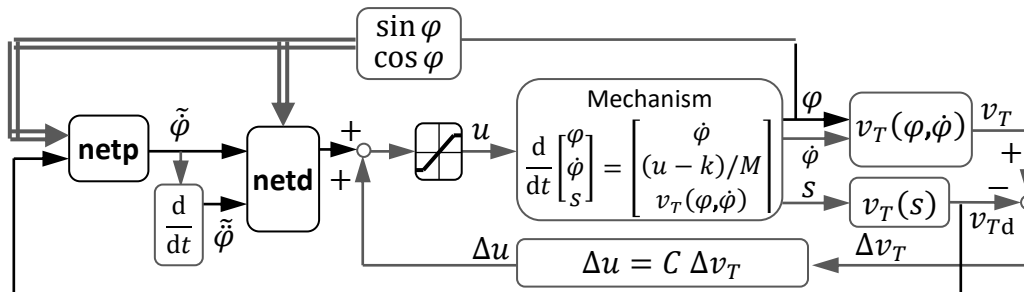
To obtain inverse dynamics, the equations of motion would have to be involved, requiring deep knowledge of the internal structure of the mechanism and sophisticated calculus. Again this is avoided by generating data with randomly chosen constant drive moment  $u^{(j)}$  and random initial conditions  $(\varphi_0^{(j)}, \dot{\varphi}_0^{(j)})$ , calculating derivatives from  $\varphi_k^{(j)}$  by central differences [2], and training a surrogate according to

$$\left( \left( \varphi_k^{(j)}, \dot{\varphi}_k^{(j)}, \ddot{\varphi}_k^{(j)} \right); u_k^{(j)} \right) \xrightarrow{\mathbf{netd}} \tilde{u} \approx u(\varphi, \dot{\varphi}, \ddot{\varphi}),$$

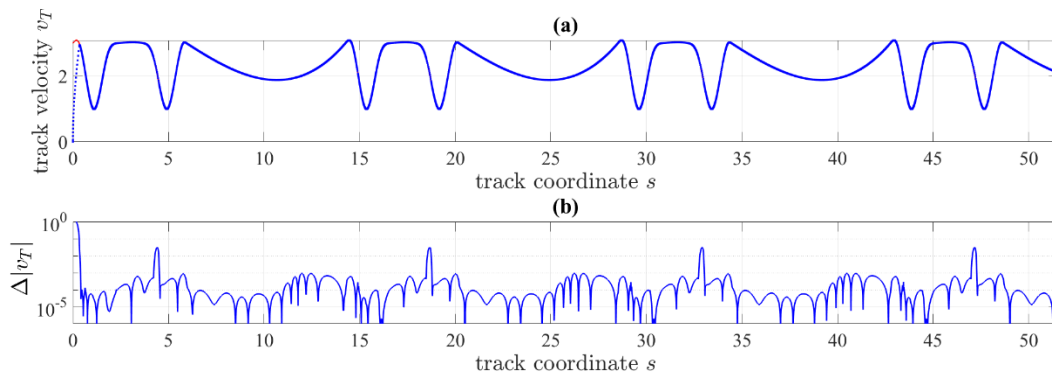
see **netd** Fig. 5. The resulting feedforward control  $\tilde{u}$  eliminates nonlinearities, which is why a simple P-controller

$$\Delta u(t) = C[v_T(\varphi, \dot{\varphi}) - v_T(s)]$$

may be used to eliminate remaining errors  $\Delta v_T(t) = v_T(\varphi, \dot{\varphi}) - v_T(s)$  between the desired speed  $v_T(s)$  and the actual track speed  $v_T(\varphi, \dot{\varphi})$  of the plant. This results in excellent accuracy with low absolute errors  $\Delta v_T(t)$  as shown in Fig. 6. It should be noted that the mechanism starts from rest, which is why it first has to accelerate and initial errors up to approximately  $s \approx 0.15$  are rather high.



**Fig 5.** Torque control of a four-bar mechanism using **netp** as inverse kinematics surrogate and **netd** as inverse dynamics surrogate for feedforward control, as well as a simple P-controller for feedback



**Fig 6.** Simulation results of the moment-controlled four-bar linkage shown in Fig 5 showing (a) desired track speed (red) and actual speed (blue) as well as (b) absolute errors

### 3. Control Design for a Lambda Robot

The above control concept is now applied to the lambda robot in Fig. 1b, see [3]. The control input  $\mathbf{u} = [F_1, F_2]^T$  combines the forces acting on the two massless sliders determining the two degrees-of-freedom  $\mathbf{q} = [s_1, s_2]^T$ . The task is to follow a desired trajectory  $\mathbf{y}_d = [x_T, y_T]^T$  of the track point  $T$ . Similar to Section 2, data is generated by classical forward simulation, where the control forces are substituted by passive spring-damper elements, see [2]. This data is then used to train inverse kinematics surrogates  $\mathbf{q} = \mathbf{q}(\mathbf{y})$ ,  $\dot{\mathbf{q}} = \dot{\mathbf{q}}(\mathbf{y}, \dot{\mathbf{y}})$  and  $\ddot{\mathbf{q}} = \ddot{\mathbf{q}}(\mathbf{y}, \dot{\mathbf{y}}, \ddot{\mathbf{y}})$ . Further, an inverse dynamics surrogate  $\mathbf{u} = \mathbf{u}(\mathbf{q}, \dot{\mathbf{q}}, \ddot{\mathbf{q}})$  is trained. Together they realize an exact feedback linearization resulting in a linear differential equation  $\dot{\mathbf{e}} = \mathbf{A}\mathbf{e} + \mathbf{B}\mathbf{u}$  for the state error  $\mathbf{e} = \mathbf{x} - \mathbf{x}_d$  between actual state  $\mathbf{x} = [\mathbf{q}^T, \dot{\mathbf{q}}^T]^T$  and desired state  $\mathbf{x}_d = [\mathbf{q}_d^T, \dot{\mathbf{q}}_d^T]^T$  obtained from the inverse kinematics surrogates. Different from the P-controller in Section 2, here an LQR concept is used to minimize the objective

$J = \int_{t_0}^{t_1} (e^T Q e + v^T R v) dt$  [4]. This results in the state feedback control law  $v = -K e(t)$  where  $K = -R^{-1} B P$  where matrix  $P$  solves the Riccati equation  $A^T P + P A - P B R^{-1} B^T P + Q = 0$ .

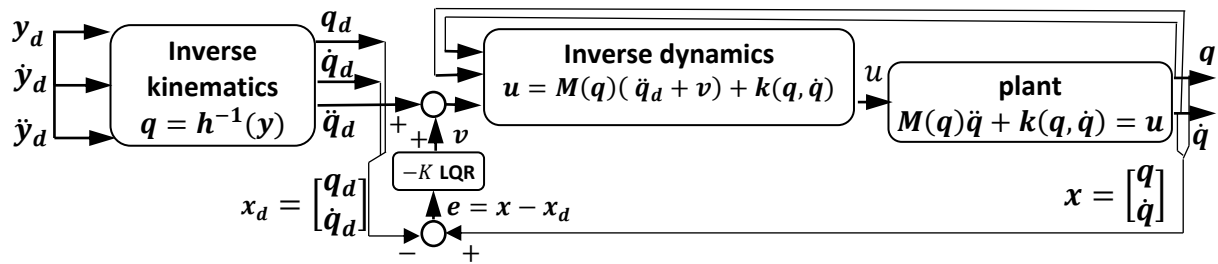


Fig 7. Control concept for the lambda robot

The simulation results in Fig. 8a indicate almost perfect performance and tracking achievement. The actual motion (blue) of the robot sliders start far away from the desired motion (red) but soon approach the desired track. Alternatively to the LQR, a PID controller may be used, Fig. 8b.

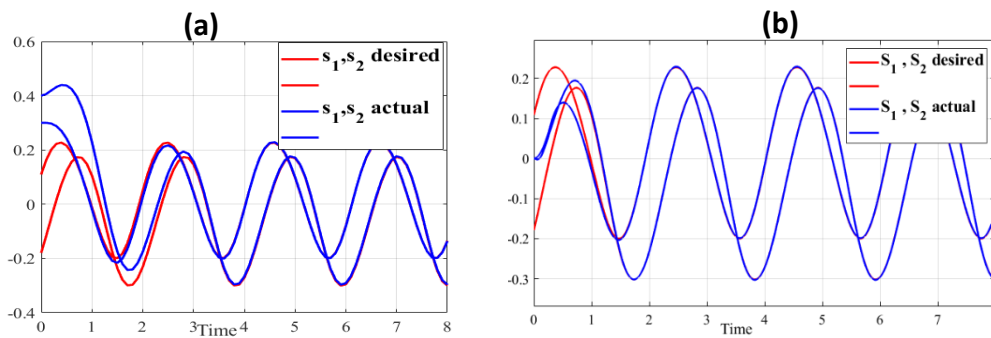


Fig 8. Simulation results for the sliders' positions of the lambda robot using a) LQR and b) PID control.

#### 4. Conclusions

The paper shows a control design concept for tracking control which substitutes human expertise by artificial intelligence. It is based purely on classical simulation of closed-loop mechanisms and shallow artificial neural networks, which provide inverse models for kinematics and dynamics to realize exact feedback linearization. Simulation results for both four-bar mechanism and lambda robot already show highly exact result for the open-loop control. An additional feedback P-controller in case of the four-bar mechanism and an LQR or PID controller in case of the lambda robot eliminates remaining errors which may result from approximation error of the surrogates, which finally results in perfect tracking.

**Acknowledgements** The project is funded by Deutsche Forschungsgemeinschaft (DFG, German Research Foundation), Project No. 501840485.

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# Event Detection and Cause Correlation for Crash Simulation Results

Dominik Borsotto

Sidact

Reaching and fulfilling several design and crash criteria during the development process is what makes the engineer adapt and redesign the simulation model over and over again. Ideally resulting in new simulation runs with in best case improved performance, matching the intention of the applied changes. For the more demanding case of unforeseen results which do not necessarily fit to the expectations of the actual changes, methods and a workflow are being introduced here, which allow to identify the root cause of this behavior.

In a first instance every new simulation run is being added into an analysis database, which is continuously being used to compare new simulations against. Previous studies have already shown that this process can assist the engineer in automatically highlighting new behavior and pin pointing the engineer to the regions of interest. Rather than only highlighting the new behavior now a second phase is being triggered additionally.

In this second phase the previously detected event is being isolated and analyzed against the gathered data of the development history. The analysis methods used are based up on the Principal Component Analysis, a reduced order modelling technique. This allows not only identifying structures in the data but also correlating deformation patterns against each other. Especially the latter one is of interest for an automated process, as it allows automatically detecting and suggesting possible root causes to the engineer. As an outcome of this process the engineer receives a list of correlating parts, so that he can focus on deriving a better engineering solution to achieve a deterministic behavior, rather than searching for the root cause of the event.

To provide additional information about the type of cause, as for example failure or buckling, the identified parts are also forwarded to a classification prototype. This type of classification shall assist the engineer in deriving a possible design adaptation.

# Machine Learning Tools for Multiphysics Analyses, Design Exploration and CAE Acceleration

D.Drougkas BETA CAE Systems SA

## 1 Summary

Machine learning tools have become increasingly prevalent in various software applications, offering numerous advantages and transforming the way we interact with technology. The challenge in the CAE-domain and Multiphysics analyses in particular, is to adapt and learn from the huge amount of Simulation data, plus demanding load cases and complex physics. The ML-workflow which involves data collection and preparation, ML-model training and evaluation, and finally Prediction.

The Prediction of scalar, 2d, 3d and Multiphysics Simulation results give us the opportunity to use Machine learning for variety of applications. Predictors as the ML-object in BETA Products enable CAE engineers to rapidly explore various design configurations without relying on time-consuming simulations. Engineers can now optimize their processes, streamline workflows and expedite the realization of innovative designs.

## 2. Parametric Multiphysics Optimization

This study aimed to optimize the design and manufacturing of the tailgate component of a vehicle on two fronts: manufacturing quality and ease of use. The process evolved around the specification of the gas lifter components mounting positions and force rating.

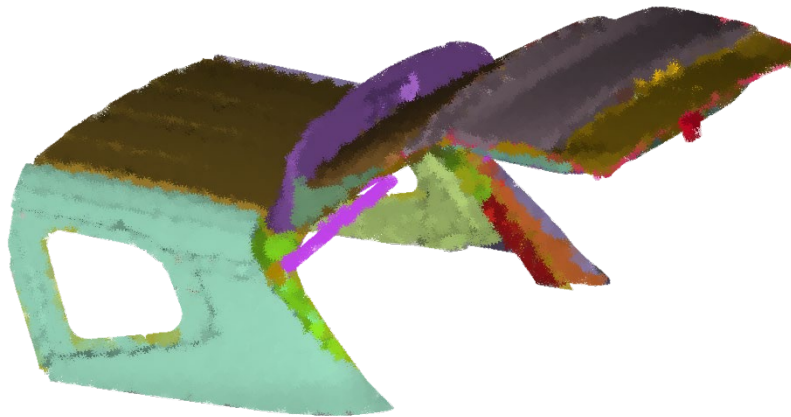


Fig. 1 Tailgate with gas lifters

To optimize these two requirements, both Multi-Body Dynamic and structural analyses were essential. The goal was to maintain the deformations of the tailgate component at reduced levels resulting in optimum external appearance regarding panel gaps, while maintaining a comfortable user operation of the tailgate.

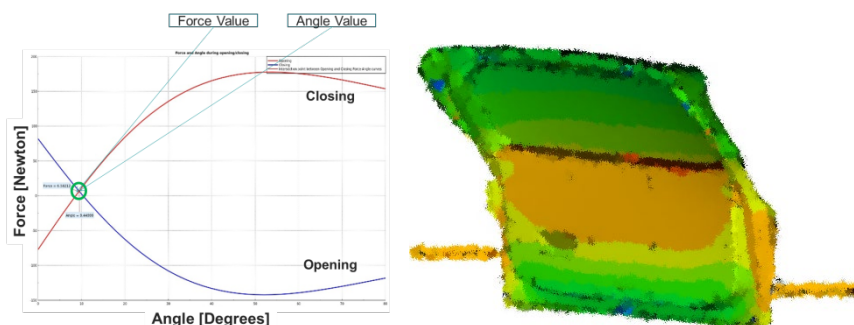


Fig.2 a. Multi Body Dynamic analysis results, b. Structural analysis results

After an initial Design Of Experiments (DOE) with 20 variations of the parametric model, Machine Learning predictive models (also refereed as predictors) were employed in order to accelerate the product design and evaluation process by predicting the two solvers results. Continuing these predictors were updated with new DOEs created by automatic smart sampling methods, in order to improve their accuracy.

Finally these Machine Learning predictors were employed in Optimization studies, replacing the two solvers, in order to reach the optimum design in an automated and faster way, thus, improving the product development time. The objectives were to minimize the deformations of the panel and minimize the force required by the user to open and close the tailgate.

**Table 1: Optimization Results with and without Machine Learning**

Optimal Design	F1	S1_X	S1_Z	S2_X	S2_Z	N555914_dx	N613869_dx	Angle	Force	Time (hours)
Initial Design (reference)	600	3388.346	963.711	3218	1203	1.4573	1.4155	9.4499	6.5821	-
Direct Optimal	400.304	3391.47	967.006	3219.88	1201.45	1.172	1.143	17.8722	0.009097	<b>157.5</b>
ML Approach	404.939	3392.924	969.289	3219.425	1201.799	0.5519	0.5189	19.017	0.7731	<b>63</b>

**2 Non Parametric Machine Learning - Body in White first torsional mode prediction**

Identifying the first torsional mode of a vehicle’s Body-in-White (BiW) marks a crucial stage in the product development. During product development, the BiW may undergo several types of modifications in its design and engineering specifications. These modifications may include changes in geometry (shape of parts), changes in parts thickness, and changes in materials or connection types. Each design modification requires the creation of a new simulation model, and then a new run of a Finite Element analysis to collect the desired responses. This iterative redesign process may need to occur several times in the development cycle of a BiW.

In this work, BiW FE models from various vehicles served as input data. This Machine Learning method, also known as Feature-Based or non parametric, utilized the actual FE models and their scalar values as input, without relying on specific parameters. The method conducted automatic feature extraction, from each FE model during training and used the extracted data as input. A total of 100 different FE models were used for training.

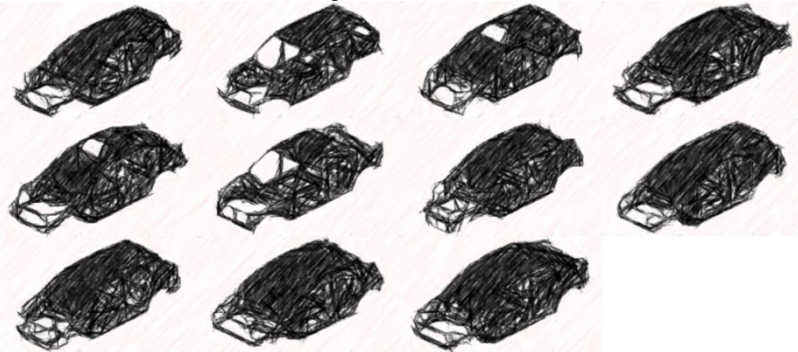


Fig.3 Various Body in White FE models used as training input

For each FE model, the frequency values corresponding to the first torsional and first vertical bending modes were identified and utilized as responses for training the machine learning predictor.

**Table 2: Labelled Responses used for training**

FE Model	First torsional value (Hz)	Vertical bending (Hz)
BiW_1	32.411	38.492
BiW_2	34.096	39.123
BiW_3	42.198	43.608
BiW_4	29.329	42.86
BiW_5	...	...

Once the Machine Learning model was trained, it offered insights into its accuracy and performance by means of metrics (Mean Absolute Error, etc) and Key Performance Indicator (KPI) plots.

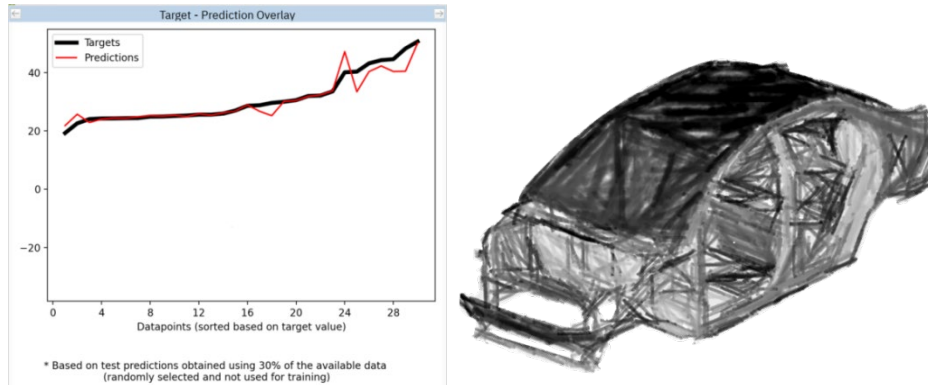


Fig.4 KPI Target vs Prediction overlay plot (left). New BiW FE model, unknown to the predictor (right.)

For any new BiW FE model variation, whether it belongs to a similar or different carline, the trained Machine Learning model can provide predictions for the labelled responses much faster than the respective FE analysis, along with the confidence bounds.

Table 3: Prediction Results and error

	First torsional value (Hz)	Vertical bending (Hz)
<b>Prediction</b>	39.74	40.88
<b>FE Result</b>	39.73	40.78
<b>Abs Error</b>	0.01	0.1

### 3 Mode Classification

Mode classification is a process used in structural analysis cases in order to analyze and label how structures deform under various loading conditions. This process is particularly used for NVH (Noise Vibration and Harshness) discipline, when performing normal modes analysis. The identification and classification of each mode shape is a demanding task and requires experienced engineers to work together to complete it. Machine Learning can be utilized in this domain, using legacy and history data to learn and provide automation in mode classification of new design variations.

In this study a dataset of different Body in White FE models were used as input data. For each model, a normal modes analysis was ran and a mode shape labeling was completed for 12 elastic modes.

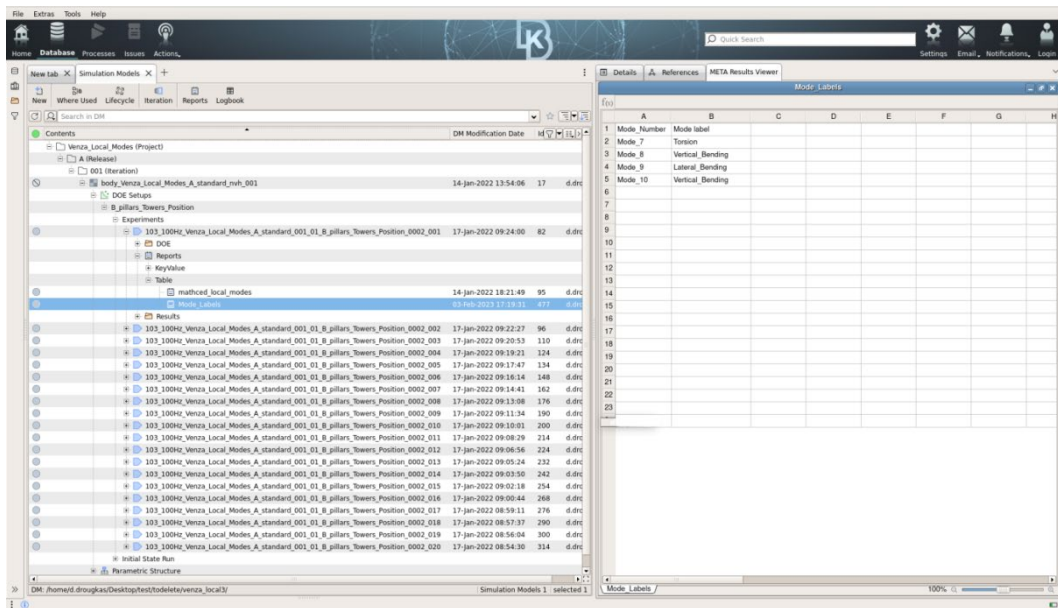


Fig.5 Training dataset for Mode classification

The trained machine learning model was used in order to predict the mode classification list, of new design variations, when provided with the normal modes analysis results.

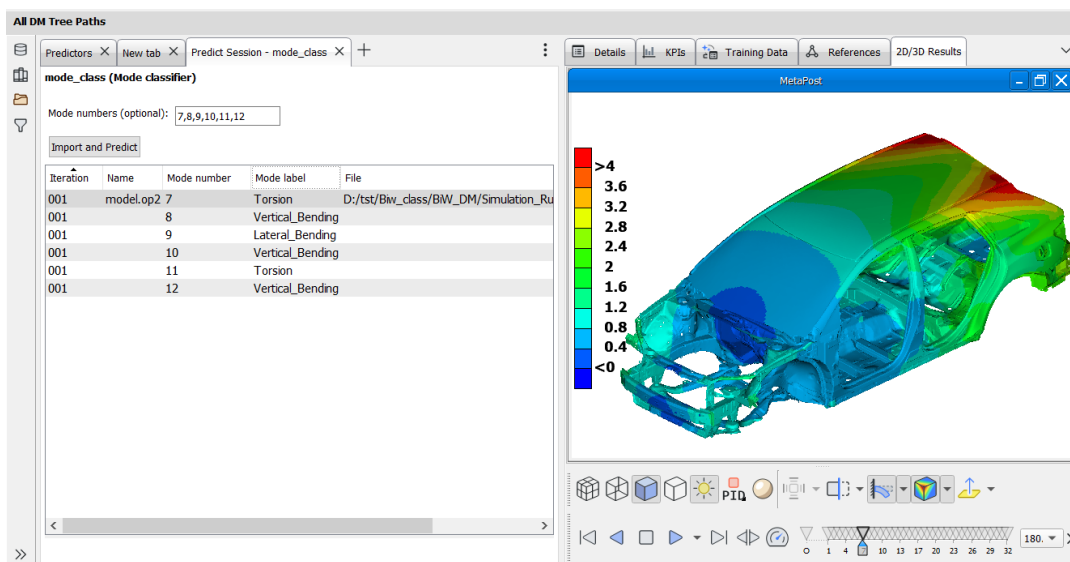


Fig.6 Mode classification prediction for new BiW variation

## 4 Conclusions

The potential of machine learning continues to grow with advancements in technology. Incorporating this functionality into CAE processes enhances the accuracy of simulation result predictions for "what-if" studies. When paired with optimization tools, it can lead to substantial time savings throughout product development. In this work, we explore the applications of result prediction in optimization, design variations, and mode classification.

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# ***AI-empowered 3D Surrogate Modelling: Case study of Thermo-Mechanical Simulation of a Glass Table***

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Barakat Bokharaie (Velux)

## **1 Summary**

Accelerated product development cycles required in today's fast-paced world present both opportunities and challenges in the present industry – demanding innovative designs, sustainable manufacturing and an enhanced product experience. This sense of urgency leads to several challenges such as: design flaws, compromised performance, and higher production costs. Moreover, this coupled with the traditional development methods, which typically involve a siloed data exchange between CAD designers, CAE simulation analysts and manufacturing experts, restricts efforts towards design optimization, therefore resulting in sub-optimal products.

To tackle these challenges, Dassault Systèmes' **3DEXPERIENCE®** platform seamlessly integrates the modelling and simulation processes through unifying the well-established CATIA® and SIMULIA® solutions widely adopted across industries. This paradigm, referred to as MODSIM, helps maintain a digital continuity between CAD-CAE experts throughout the development process. This promotes avenues for easier parametric model development, simulation-driven design optimization, and Design of Experiments (DoE) based data generation. Furthermore, leveraging this generated DoE data, our latest machine learning and AI-driven simulation techniques can act as surrogates to physics-based simulations. This enables accelerated simulation predictions, and therefore a rapid data-driven discovery of optimal design alternatives.

In this work, through a collaborative use case with VELUX, we demonstrate how data-driven AI-empowered MODSIM on the **3DEXPERIENCE®** platform helps accelerate thermo-mechanical simulation of a glass table. We demonstrate fast executing neural networks which are trained as 3D surrogates using parametric DoE data (ranging across table geometries, loads and materials) generated from physics simulations. Trained models are then deployed in a collaborative design environment for rapid exploration. This allows designers to evaluate numerous parameters within a vast design space, thereby enabling robust optimized products. By delivering high-fidelity physics predictions, which cover both transient responses and 3D fields (temperatures/displacements), this proposed technique can significantly enhance the efficiency of science-based product development. By embracing this systematic and collaborative approach on the **3DEXPERIENCE®** platform, coupled with the efficiency of AI-empowered surrogate modelling technology, industries can navigate the complexities of swift timelines while ensuring the delivery of optimized, sustainable and innovative products to the market.

## **2 Simulation Model and DoE Setup**

In this work, we collaborate with VELUX on a ML-driven thermo-mechanical assessment of a glass table. The Glass Table model setup is parametric; and includes geometric, loading and material variations. The geometric parameters include features of the table such as table-leg length, glass and frame thickness, etc. The glass table is subjected to a temperature difference across the opposite glass faces, and then to a subsequent pressure load by the user. Temperature difference (30C, 50C, 70C) across the glass is a variable loading parameter. Finally, the frame of the glass table is considered to be made of two different elasto-plastic materials (Aluminum or Steel).

The use case targets ML-driven prediction of how the applied structural loads, and a temperature difference across the glass accrue deformation in the glass table. Therefore, this was performed as a sequential thermal-structural simulation using the ABAQUS® solver. First, the thermal conductivities of the different materials were assigned, and a steady-state thermal simulation was performed. As a result of this simulation, nodal temperatures in the model are calculated as output. Using this information, a subsequent non-linear structural simulation is set up, accounting for the pressure load applied on the top of the glass table. The output of the structural simulation includes displacements, strains and stresses.

Fig. 1 shows the table geometry and the different materials considered in the model, while Fig. 2 shows the different geometric parameters considered. Fig. 3 shows the loading setup. Finally, Fig. 4 shows the overall scope of this ML use case.



Figure 1: Glass table geometry and the materials applied to different parts

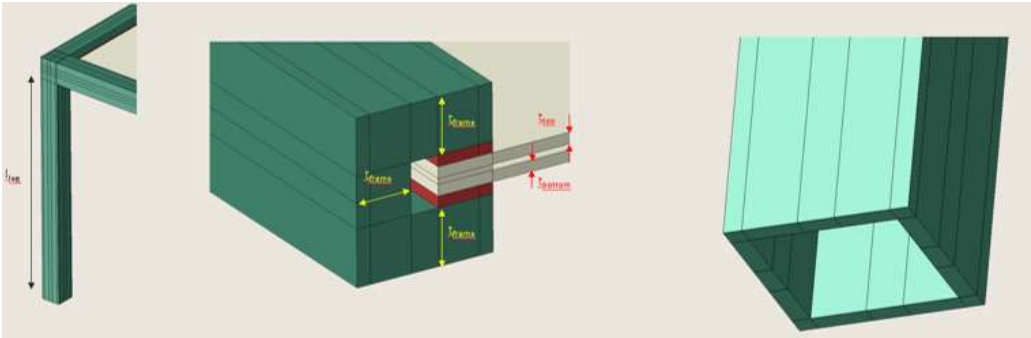


Figure 2: Geometric parameters of the glass table geometry

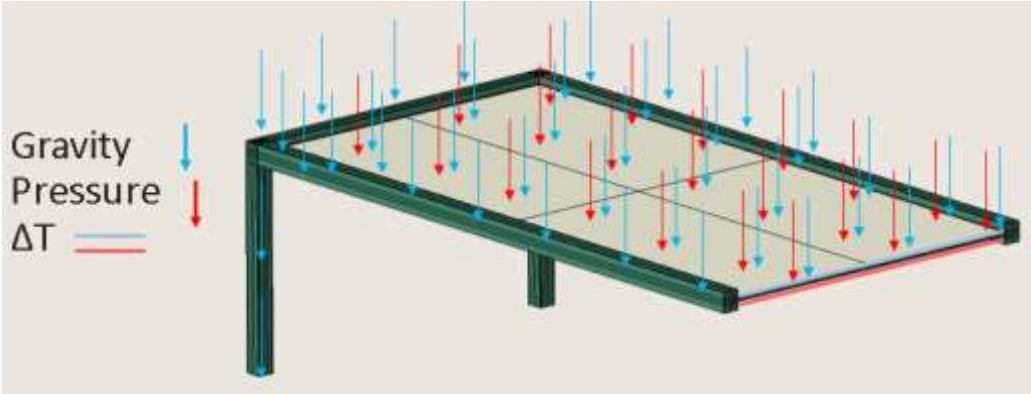


Figure 3: Loads considered for the sequential thermal-structural simulation of the glass table

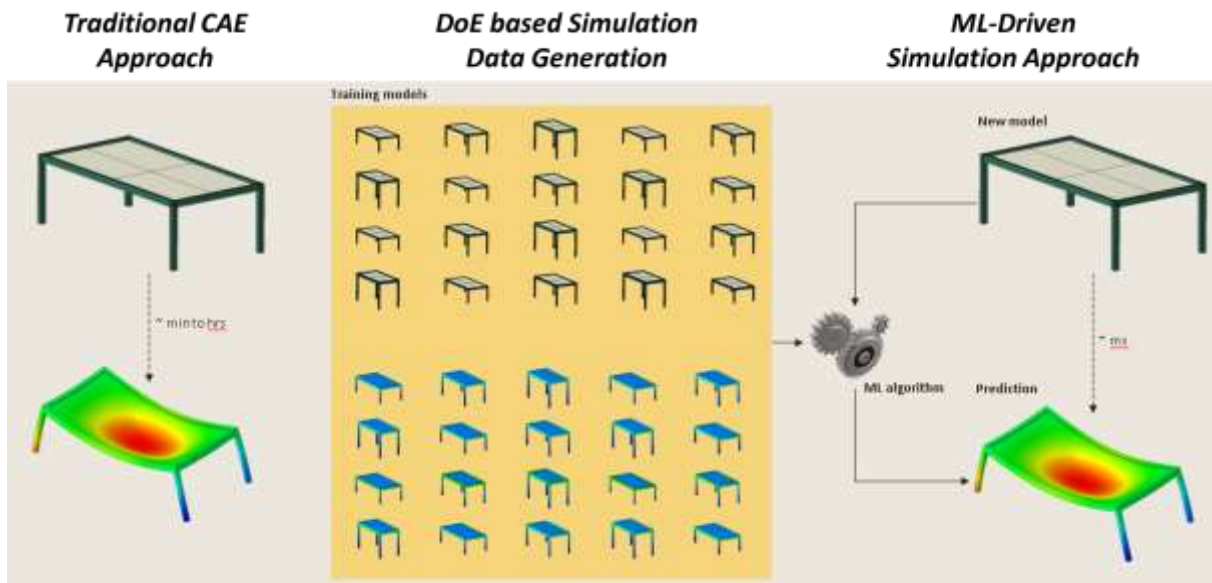


Figure 4: Scope of this ML-driven simulation use case

As shown in Figure 4, we first prepare a Design Space which consists of a range of different design points from the parametric space consisting of 4 geometric variables, 3 loading temperatures, and the 2 materials of the frame as shown above in Figure 2. By randomly picking the values of these parameters, we choose different spans of the design space from 20-60. The 3DEXPERIENCE platform has dedicated apps, like Optimization Process Composer for creating and running such DoEs, where several advanced design space generation techniques can be used, like Sobol Sequence, Latin Hypercube, etc. The simulation data from this DoE is stored, and the displacements at all nodes in the glass from the structural analysis are extracted to train a ML model. Using this data, we train a ML model to map this displacement field in the glass in the structural analysis as a function of the 10 input parameters.

To perform this ML training, we choose 90% of the samples of the DoE for training, and keep the remaining 10% samples for blind validation. We assess the ML prediction on these blind validation samples. Once trained, the displacement field predicted from the ML model corroborates accurately (<5%) with respect to the displacement field predicted from the high-fidelity ABAQUS® based simulations. The number of training runs required to establish good accuracy of the ML model were tested by varying the DoE size between 20-60 simulations.

The ML prediction, on a GPU card runs upto 250 times faster compared to the time required for a similar thermal-structural model run based on a single CPU ABAQUS® simulation.

## Conclusions

In this work, we performed a DoE for a complex multi-physics simulation involving a sequential thermal-structural analysis of a glass table. The DoE was conducted to create a design space comprising of a large number of design points (20-60). Using this DoE data, we train a ML model by choosing different number of training samples. Validation is performed on 10% of the design space. The trained model is able to accurately predict the full field of displacements, upto 250 times faster. This framework can therefore be leveraged to make rapid design changes in the geometric/loading or material parameters, and visualize ensuing deformations in the glass table in real time. By extension of this framework, the glass table design can be optimized to minimize glass deformations as a function of the given input parameters.

Through such an integrated modelling-simulation approach on the 3DEXPERIENCE® platform to generate multi-physics DoE data, coupled with the efficiency of our AI-empowered surrogate modelling technology, industries such as VELUX can swiftly apply these ML-trained surrogates based on advanced physics simulations to swiftly make predictions on design components, while ensuring the delivery of optimized, sustainable and innovative products to the market.

# Memory for Your AI: Lessons learned from 6 years of applied research on contextual graph-data-bases as enabler for AI use cases

Christopher Woll (GNS Systems GmbH), Marco Lah (Context64.ai GmbH)

## 1 Current Situation

Today, and in the coming years, companies in all sectors are facing the major challenge of managing the data resulting from the rapid advance of digitalization. According to estimates by the international market research and consulting company IDC [1], the amount of data worldwide will increase to up to 284 Zbyte by 2027. And there is no end in sight to the flood of data. Companies are therefore already improving their competitive position by making more efficient and intelligent use of the data they collect, by collecting new data in a more targeted manner and by using advanced intelligent analysis methods, see the Lünendonk study "From data silos to data streams" [2] from 2022. The aim should be to bring together and efficiently process data from a wide variety of sources and processes to use it effectively.

However, current practice and a representative survey of 603 companies from all sectors of the economy commissioned by the digital association Bitkom in 2024 show a different picture: Data remains unused in most German companies [3]. 60 percent of the companies surveyed stated that they are exploiting the potential of their data little or not at all. Only 6 percent assume that they are fully exploiting the potential of the data available to them. There are many reasons why data is unused in companies - in Germany and around the world. Data is often interpreted in its own way due to different responsibilities, specialist knowledge and contextual relevance and used for the development of innovative products, for example.

With the shift to a data-driven corporate culture, the demands on data management are also increasing. The use of information of all kinds requires the dismantling of data silos and the provision of new tools to create uniform access to data and eliminate fragmented data interpretations. Modern methods and the use of artificial intelligence have become significantly more important in recent years to efficiently process data in simulation-driven design. Generative AI models have increasingly become the focus of interest for companies.

While AI can use machine learning to make number-based decisions and predictions based on data and algorithms, GenAI can use training data to independently create new content such as text, images and audio. One of the most prominent examples of this is ChatGPT. Based on a Large Language Model (LLM), the chatbot can communicate with users via text-based messages and images. Eight out of ten companies are already using generative AI technology to carry out data analyses, interpretations and forecasts, according to the Lünendonk study "Generative AI - From innovation to market maturity" 2024 [4]. 80% of the companies surveyed in the study "Harnessing the value of generative AI 2nd edition: Use cases across sectors" 2024 [5] by Capgemini even stated that they had increased their investments in the technology compared to the previous year. These extensive investments are driven by the far-reaching increases in efficiency and productivity that companies are aiming to achieve through the introduction of generative AI, as summarized in the quarter three report "State of Generative AI in the Enterprise" [6] by global management and strategy consultancy Deloitte.

As a data integration and management platform, the Data Context Hub (DCH) addresses current challenges in handling data and uses context-enriched information to provide companies with holistic market insights for faster, cost-efficient product development. The scalable platform, which was developed as a research project over 6 years at Virtual Vehicle Research (Graz) together with automotive and rail OEMs, uses both state-of-the-art methods and artificial intelligence models.

## 2 DATA CONTEXT HUB: Transform data into competitive advantage

Through AI-supported contextualization, DCH enables companies to seamlessly transform raw data into structured, actionable knowledge. Since data, as already described at the beginning, only achieves

optimal benefit when it is not available in isolated silos, the DCH breaks down existing structures by using a networked, accessible format. The platform brings together information from R&D and production data sources as well as from telemetry data streams or storage locations such as data lakes. The DCH then creates an explorable context map in the form of knowledge graphs from area-specific data models. Due to their flexible and scalable structure, these knowledge graphs are ideally suited to reflect the inherent relationships of the different data types. This is done by applying a semantic layer that connects the data points according to defined rules. The resulting context between different data points intuitively clarifies the relationships between information and reduces the risk of fragmented data interpretations. The concept behind DCH is therefore essential for streamlining processes and reducing risks.

## **2.1 Boost decision-making with context**

The embedding of corporate knowledge in a coherent structure facilitates precise, context-driven data access and supports the company's requirements for a standardized, adaptable knowledge system. The DCH thus allows engineers to quickly retrieve complex, multidimensional knowledge in a repeatable manner via a single platform and use it for the data-driven development of innovative products. In addition, the data analyses created are based on a coherent, context-related foundation.

## **2.2 Easy access to generative AI**

The use of modern AI models in DCH also supports engineers in gaining deeper insights from the data, predicting trends and automating tasks. It is possible to integrate generative AI in the form of large language models (LLMs) into the process of interpreting knowledge graphs. This works as follows: In the first phase, a defined data model searches a large dataset for relevant information. Retrieval augmented generation models (RAG) used in the following phase optimize the initial search. GraphRAGs use vector embeddings to represent the data. The model thus identifies relevant information based on semantic similarity and not by searching for exact matches. The information retrieved in this way then flows into the subsequent generation process.

By utilizing specific, retrieved information, the RAG models can provide more accurate and detailed answers. Using the generative models focuses the retrieved information on the context rather than generating it from scratch. The fast response times also support a wide range of sources and data to be retrieved in the shortest possible time. LLMs trained on the GraphRAG-enhanced knowledge graph thus efficiently uncover patterns, predict trends and suggest optimizations for tailored workflows.

## **3 Insight into practice: Mastering complex, data-intensive challenges with DCH**

The scalable platform was developed as a research project for over 6 years at Virtual Vehicle Research (Graz) together with automotive and rail OEMs. The following two practical examples from the automotive and manufacturing industries show how the Data Context Hub supports companies in transforming complex data into clear, actionable insights.

### **3.1 Use Case 1: Virtual buildability checker for automotive OEM**

The automotive sector is characterized by high complexity in product configurations, driven by customer demands for customized features and the need to comply with diverse regulatory standards across global markets. For a leading automotive OEM, the challenge was to evaluate buildable vehicle configurations among an enormous array of possible options. Traditional tools and methods proved insufficient due to the exponential number of potential combinations, which led to extended simulation times and manual configuration checks, slowing down the development cycle.

The solution lay in leveraging the DCH platform to create a Virtual Buildability Checker, specifically designed to capture, simplify, and query complex configuration dependencies. Through DCH's knowledge graph, we represented the configuration rules as nodes and relationships in a directed graph structure, encapsulating complex dependency rules into simpler logical constructs.

The platform's flexible data collection layer enabled the creation of a custom data import provider tailored to the client's individual configuration rules. This provider extracted and organized relevant data, representing rules such as graph nodes and relationships that depicted dependencies among various components. For example, options in vehicle configuration that affected component compatibility were stored as connections within the graph, facilitating rapid and accurate determination of buildable configurations.

Beyond the core configuration data, DCH's architecture also made it possible to enrich the graph with additional context, such as simulation parameters, CAD geometries, and supplier details.

By querying this interconnected data through DCH's intuitive API, the client's development team could access integrated data insights and quickly verify buildable configurations against external criteria. This solution reduced the client's engineering development time, accelerating frontend application delivery for internal engineering use by enabling rapid, data-driven decision-making and reducing dependency on manual configuration validations.

### **3.2 Use Case 2: Knowledge graph as memory for AI models**

In another application, DCH was employed as a foundational memory system for enhancing AI-driven insights through Generative AI models, particularly Large Language Models (LLMs). This approach aimed to leverage both internal and external data sources in a structured, interconnected knowledge graph, thereby enhancing the AI's contextual understanding and ensuring precise responses aligned with real-world, data-informed knowledge.

DCH's knowledge graph provides a holistic data structure where connections between nodes capture and reflect various contextual relationships critical to the client's business needs. By linking internal data sources - such as PLM, PDM and Requirements Management tools - with external data sources, including user feedback and product performance data, DCH allowed the client to gain nuanced insights that were previously inaccessible in siloed environments.

The DCH module, "Memory for Your AI" (M4AI), enables users to specify queries in the form of natural language prompts. The M4AI context-building engine dynamically navigates the knowledge graph to create coherent networks of relevant information nodes, supplying the Generative AI model with accurate, context-rich inputs. This approach eliminates "hallucinations" in AI responses, a common challenge in LLM applications, by grounding the outputs in factual, interconnected data points. Each AI-generated response is accompanied by a traceable path within the graph, detailing the data sources and relationships that contributed to the final answer, thus providing transparency and fostering user trust.

The client employed this M4AI-powered system to analyze user feedback and field data, uncovering new opportunities for product improvement and service enhancement. By aligning AI-driven recommendations with customer insights and operational data, the DCH-powered AI system enabled actionable insights and rapid responses to emerging trends. This use case highlights the DCH platform's capacity to transform data-intensive AI applications by establishing a structured, context-aware foundation for information retrieval and decision support.

## **3 Conclusions**

The contextual graph databases of DCH already offer an important approach for technical use cases in practice. The underlying concept combines the ability to retrieve information from a large database with the generative capabilities of state-of-the-art AI technologies such as LLMs in a forward-looking way in the field of simulation-driven design.

Driven by an accelerated pace of innovation, companies today face the major challenge of bringing products and services to market cost-effectively, qualitatively and in ever shorter development cycles. The Data Context Hub (DCH) can support companies in providing relevant data in an easily accessible, context-related format in a centralized and organized manner to meet the new requirements of volatile markets in a future-oriented manner.

High flexibility in handling the data - from conceptual ideas to production - allows engineers in all industries to quickly obtain cost forecasts, competitive analysis, trend monitoring, risk assessments and historical knowledge from the information. The platform's concept of using knowledge graphs enables efficient data retrieval and supports short validation and iteration cycles, which are essential for maintaining competitive advantage in demanding engineering environments.

The concept behind the DCH offers a future-oriented approach to managing and using information. It lays the overall foundation for smarter, faster and more accurate engineering decisions. DCH's ability to integrate disparate data sources into a coherent, accessible knowledge base offers companies a way to optimize their operations, shorten product development times and improve decision-making

processes. Providing an optimized knowledge management interface and AI-powered storage system enables engineers to explore ideas, validate innovations and bring them to market faster. DCH provides engineers with a future-oriented, data-driven tool that allows them to innovate confidently and efficiently, closing the gap between raw data and actionable insights.

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# Applications of AI/ML in Fatigue Analysis

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# Automated Damage Localization in Carbon Fiber Composites via Machine Learning and Deep Learning

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## 1 Abstract

The increasing use of composite materials in key industries like automotive and aerospace has intensified the focus on Non-Destructive Testing (NDT) and damage detection techniques for these components. In this context, optical measurement techniques, such as Laser Doppler Vibrometry (LDV), offer an effective experimental setup for obtaining measurements from dense point grids without adding mass to the structure. In order to analyze the large measurement campaigns with high-frequency vibration data for defect classification, Machine Learning (ML) and Deep Learning (DL) techniques hold significant promise for developing reliable and automated frameworks. In this study, various ML and DL methods were evaluated for detecting defects in a Carbon Fiber plate using frequency response data. These approaches were enhanced by incorporating simulated datasets generated through Finite Element Analysis (FEA) within a Transfer Learning framework. Since simulation data is easier to produce than experimental data, any benefits gained from its use are advantageous. The results of the damage detection process are detailed, along with a comparative analysis of the different techniques employed.

## 2 Introduction

Composite materials, consisting of distinct phases like matrix and fiber, offer a superior strength-to-weight ratio, high tensile strength at elevated temperatures, and fatigue resistance, making them essential in industries such as automotive [1] and aerospace [2]. With their increasing application, innovative methods for damage monitoring are in demand. Non-Destructive Testing (NDT) techniques, especially Laser Doppler Vibrometry (LDV), enable high-frequency analysis of materials without affecting their integrity, aligning with the Local Defect Resonance (LDR) concept [3] to facilitate defect detection by targeting local stiffness reductions. Machine Learning (ML) further supports this by automating damage detection through feature engineering, while Deep Learning (DL) techniques provide end-to-end approaches on raw data, proving effective across various applications, including composite materials [4] and machinery [5].

This paper explores damage detection in composite structures, beginning with Laser Doppler Vibrometry (LDV) measurements on a Carbon-Fiber Reinforced Polymer (CFRP) specimen. Next, ML and DL algorithms are applied to develop three detection methods: the Convolutional Neural Network (CNN), the Anomaly Detection Autoencoder (ADAE), and the Autonomous Anomaly Detection (AAD). Simulation data is incorporated through Transfer Learning (TL) to enhance the CNN's performance. The paper provides a description of each step within these methodologies and presents a comparative analysis of their effectiveness.

## 3 Experimental setup

A series of measurements were conducted with an Optomet SWIR Laser Doppler Vibrometer (LDV), a contactless method leveraging the Doppler effect to measure vibration velocity without mass loading, unlike traditional instruments like accelerometers. The test subject was a 5.43 mm thick Carbon Fiber Reinforced Polymer (CFRP) plate with Flat Bottom Hole (FBH) damages. The LDV was positioned vertically above the undamaged top surface of the plate, which was supported by foam, and excitation was provided by a piezoelectric (PZT) patch attached to the plate's underside. To trigger resonance associated with defect vibrations, the plate was excited up to 80 kHz using a chirp signal from the

LDV's generator, amplified 50 times by a Falco Systems WMA-300 amplifier. Figure 1 shows the setup.



Figure 1: LDV experimental setup

The CFRP plate consists of 24 laminae with a [(45/0/-45/90)]<sub>3s</sub> stacking configuration and includes 12 defects of varying size and thickness. The measurement of plate was split into two halves, from the middle of the specimen, and the top half served as the test subset for the damage localization algorithms.

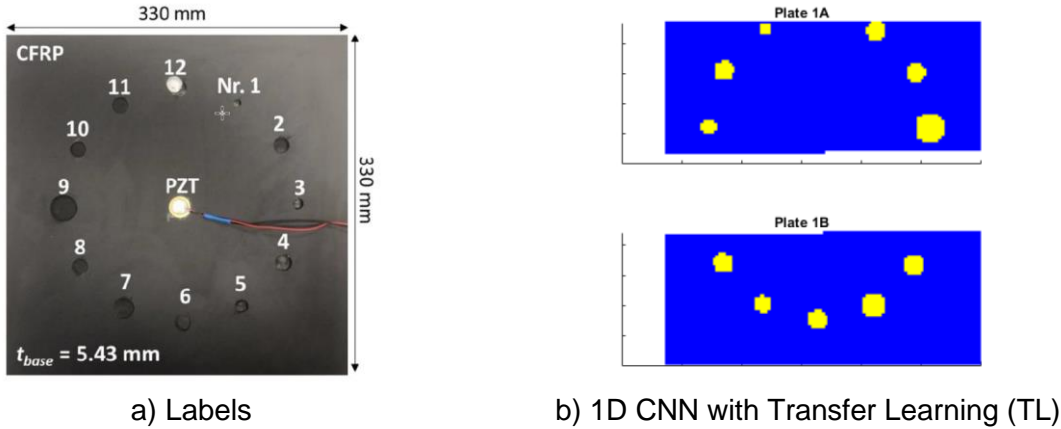


Figure 2: Test specimen - Carbon-Fiber Reinforced Polymer (CFRP) plate. The top section of the plate (Plate 1A) was used as the test subset of data for the damage localization algorithms.

#### 4 Analysis

Beginning with vibration data collected by the LDV in the previously described experimental setup, various methodologies were created to locate damage on the test specimen. These methods consist of several phases: pre-processing, feature selection, machine learning techniques, and post-processing. A color-coded schematic in Figure 3 illustrates the sequence of each stage in the damage detection methods. In terms of machine learning, three algorithms form the foundation of these approaches: the 1D Convolutional Neural Network (1D CNN), the Anomaly Detection Autoencoder (ADAE), and the Autonomous Anomaly Detection (AAD). Notably, each algorithm represents a different type of learning approach—supervised, semi-supervised, and unsupervised learning, respectively. These techniques were developed concurrently and iteratively to provide a comparative evaluation of each learning type in addressing the damage detection challenge.

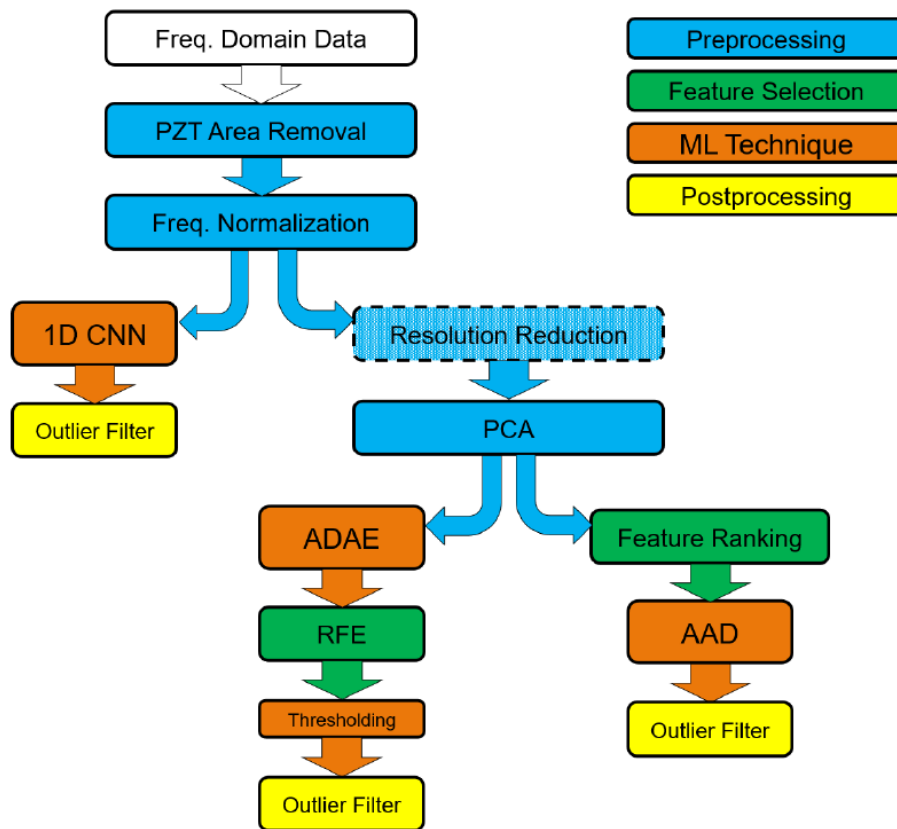
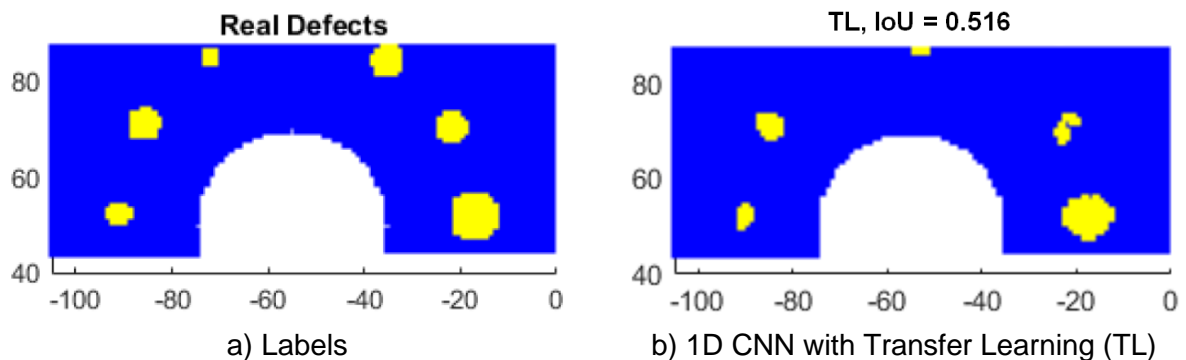


Figure 3: Damage localization methodologies

The results are shown in Figure 4. The 1D CNN demonstrated the highest Intersection-over-Union (IoU) score, highlighting its accuracy in identifying damaged areas. While the ADAE successfully detected four damages (along with the manufacturing error), similar to the 1D CNN, it was less precise in localizing these areas. The AAD detected one additional damage correctly, however, it also detected false positives, as indicated by the smaller yellow regions near the damage in the bottom right corner of the results.



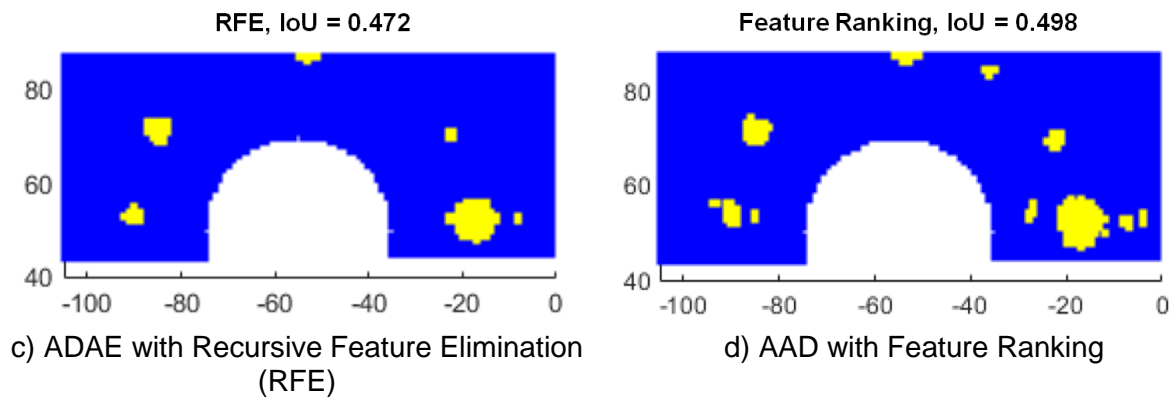


Figure 4: Damage localization results for the three algorithms.

## 5 Conclusions

This study investigated various ML and DL techniques for defect detection, covering algorithms in supervised, semi-supervised, and unsupervised learning domains. Each method was fine-tuned for optimal hyperparameters, and simulation data was utilized in a Transfer Learning (TL) setup to enhance the 1D CNN's performance. The 1D CNN yielded the highest Intersection over Union (IoU) score, though results showed some inherent variability. TL notably improved this algorithm's outcomes. However, the need for labeled data in supervised learning posed a limitation, impacting the 1D CNN more than the semi-supervised ADAE and the unsupervised AAD techniques. While ADAE detected the same number of defects as the CNN, Recursive Feature Elimination (RFE) enhanced its accuracy. The AAD method identified one additional defect but showed minor misclassifications, with Feature Selection further improving its outcomes. The smallest defect remained undetected, potentially due to the measurement frequency not reaching a sufficient level to activate it, as suggested by the Local Defect Resonance (LDR) concept. Future work will involve higher-frequency measurements and an expanded use of simulation data to boost accuracy, along with an extension to detect various defect types using semi-supervised and unsupervised learning approaches.

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# Artificial neural network as a surrogate to calibrate a proposed hardening model

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## 1 Summary

In the packaging industry, High-Density Polyethylene (HDPE) is commonly modelled using an elastic-plastic constitutive law with isotropic hardening due to the computational efficiency and simplified representation. However, traditional hardening models fail to capture the complex mechanical behaviour of HDPE, particularly under stable neck initiation and propagation during the deformation. To address this limitation, we propose an improved hardening model for HDPE and utilize an artificial neural network (ANN) as a surrogate for numerical material model calibration. The ANN is trained on an extensive dataset consisting of virtual hardening parameter sets and their corresponding force-displacement (F-D) responses generated via finite element simulations of virtual uniaxial tensile tests. By applying curve-fitting techniques and partitioning of the overall mechanical material response curve, we reduce the highly nonlinear F-D responses to a lower-dimensional representation, enhancing computational efficiency. The calibrated hardening model demonstrates excellent predictive accuracy, enabling instant calibration for various HDPE grades with differing properties based on simple experimental uniaxial tensile F-D data. This approach provides a robust and efficient solution for modelling the mechanical behaviour of HDPE, improving material model calibration efficiency and simulation accuracy.

**Keywords:** Artificial neural network, Constitutive modeling, Finite element simulation, HDPE, Surrogate model.

## 2 Introduction

During the last decades the Finite Element Method (FEM) has been more frequently introduced and used in the packaging industry as a complement to Computer Aided Design (CAD). Computer-based simulation models with realistic results, often referred as “virtual twins”, are used early in the development process today to ease and facilitate development and decision making in the concept and design phase. Furthermore, the simulation models are predictive at a subsystem level, macroscopic application level and lately on a microscopic level. Hence multiple length scales are nowadays involved and included in the simulation models [1].

Simulation driven package design workflows are today utilized in the packaging industry, cf. Figure 1 below. HDPE studied in this work is a material that is widely used in the packaging industry today, making it crucial to understand its properties as well as how to model them. Traditional calibration methods involve iterative adjustments of material parameters in FE solvers until experimental and simulation data align, which is resource-intensive and often limits the calibration to simple material models [2].

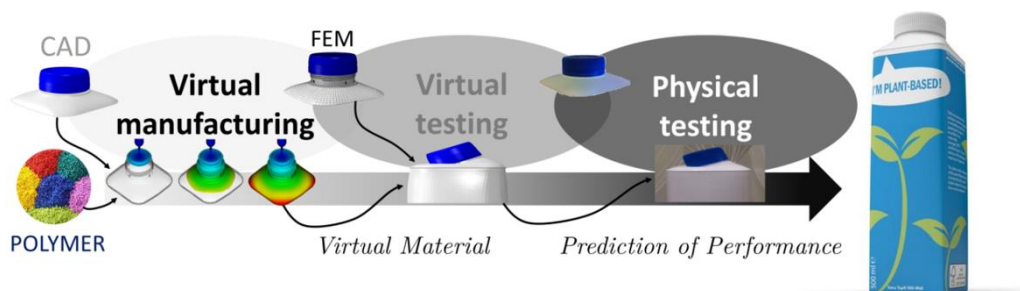


Fig. 1 Package Simulation workflow, consisting of both physical and virtual activities, Virtual Package Laboratory 2024 [3].

In this study we have built upon our experience in experimental and virtual testing and integrated the machine learning approach in our existing package simulation workflow for material model parameter identification [4].

### 3 Data-driven material characterization

The calibration process started with uniaxial dogbone tensile tests in three material orientations ( $0^\circ, 45^\circ, 90^\circ$ ) of HDPE to collect physical force-displacement and strain data. Finite element models of these experimental tests were developed in Abaqus that used a proposed hardening model and Hill48 yield criterion. Python scripts and Abaqus Isight was used to automate large enough database generation for ANN training which was trained in Matlab. The automated data generation process consisted of five main steps: **1. Initial Parameter Estimation:** Initial estimates of proposed material hardening model (as in Figure 2, total 7 parameters  $C_{1-7}$ ) and 3 yield criterion parameters were derived from experimental stress-strain curves. These estimates provided a starting point for the subsequent parameter optimization. **2. Design of Experiments (DOE):** The Abaqus Isight DOE module systematically sampled the design space defined by the material parameters of the hardening and yield models using the Latin hypercube sampling technique. This approach ensured a comprehensive exploration of the parameter space that was determined through in-depth parametric study. **3. Material Card Generation:** A Python script was developed to convert the DOE-generated parameters into material cards for Abaqus. These cards included definitions of plastic stress-strain curves and Hill48 parameters, along with constant values for Young's modulus and Poisson's ratio. **4. FE Simulations:** The material cards were used to conduct FE simulations in Abaqus. Each simulation provided detailed force-displacement and strain data for the different material configurations. **5. Post-Processing:** The output data from the simulations, including force-displacement curves and strain fields, were extracted and stored as text files. This dataset formed the basis for training the ANN.

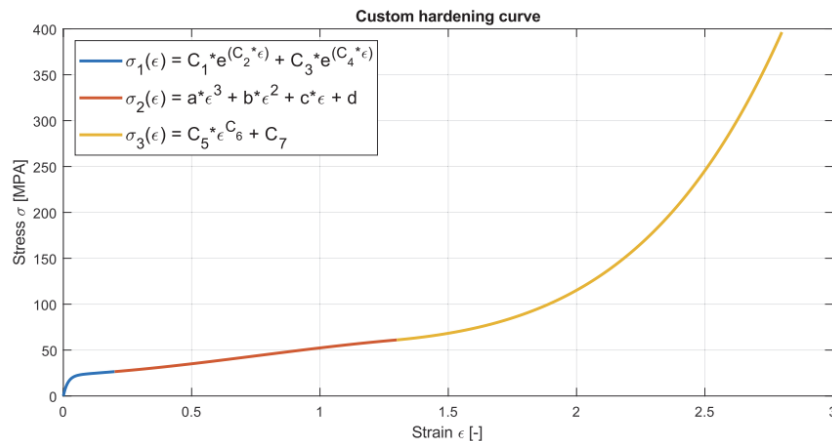


Fig. 2 Proposed hardening model and parameters in each segment [4]

The primary type of ANN used in this study was the feedforward neural network (FFNN), a well-established architecture for regression tasks [5]. Two Hyperparameter optimized networks namely FFNN1 for calibration of both hardening and yield parameters, FFNN2 for calibration of only hardening parameters were trained. Schematic illustration of the of the FFNN based calibration approach is depicted in Figure 3 that has three main stages including validation of the network.

1. Data Preparation: The input data from the FE simulations, including force-displacement and strain, were preprocessed, fitted with polynomials and normalized to ensure compatibility with the ANN. The output data, consisting of material parameters, were similarly normalized.
2. Network Training: The FFNN was trained using the prepared dataset with training/ validation/ test with 85%, 10% and 5% data. Different network configurations were explored to identify the optimal architecture for each application case. The training process involved minimizing the mean squared error (MSE) between the predicted and actual material parameters.
3. Validation: The trained FFNN was validated using experimental data to assess its accuracy and generalizability. The network's performance was evaluated based on its ability to predict material parameters from experimental force-displacement and strain data.

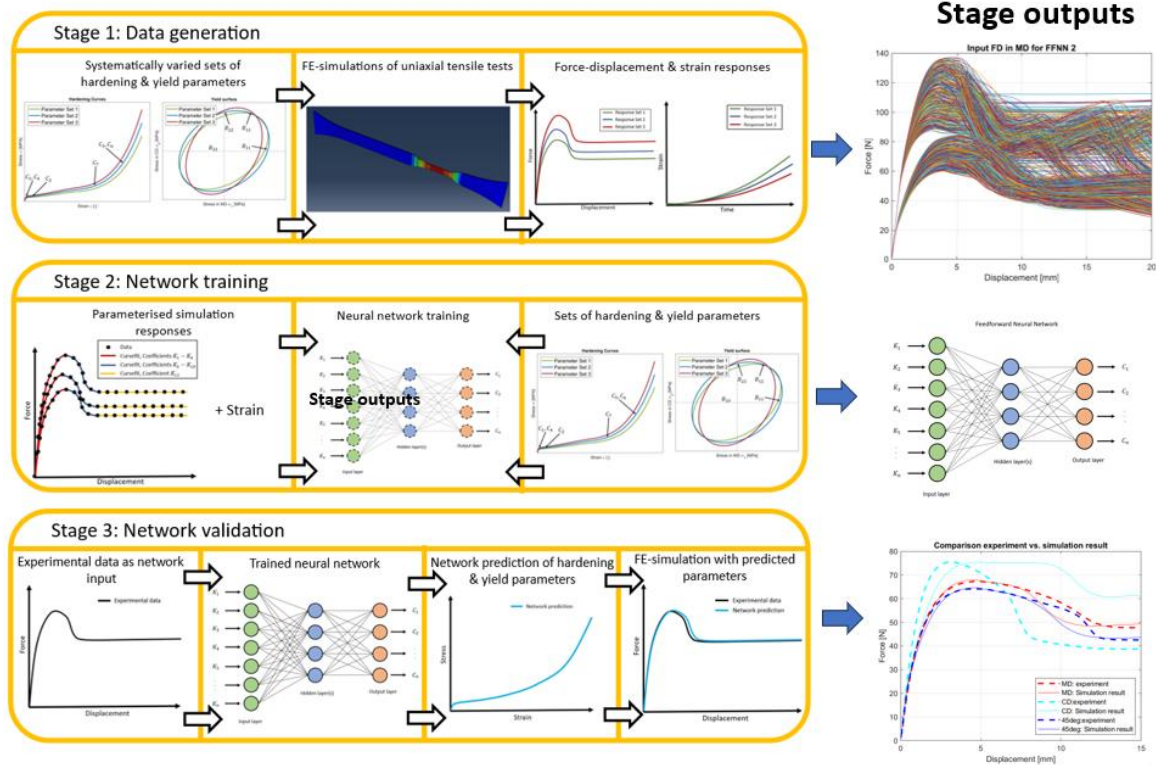


Fig. 3 Schematic illustration of the FFNN based calibration approach [4]

#### 4 Results and Discussion

In most of the studies, a total of 1000 training sets were generated to train FFNN2. Multiple datasets were used to train the same architecture. The best predicted results of FFNN2 can be seen in Figure 4 and 5. Here Figure 4 shows comparison of simulated and experimental deformation results during few selected loading sequences and Figure 5 shows the optimized hardening curve, optimum parameters and F-D comparisons. The FFNN1 performed worse than FFNN2, same is true when local strain measurements were used for training.

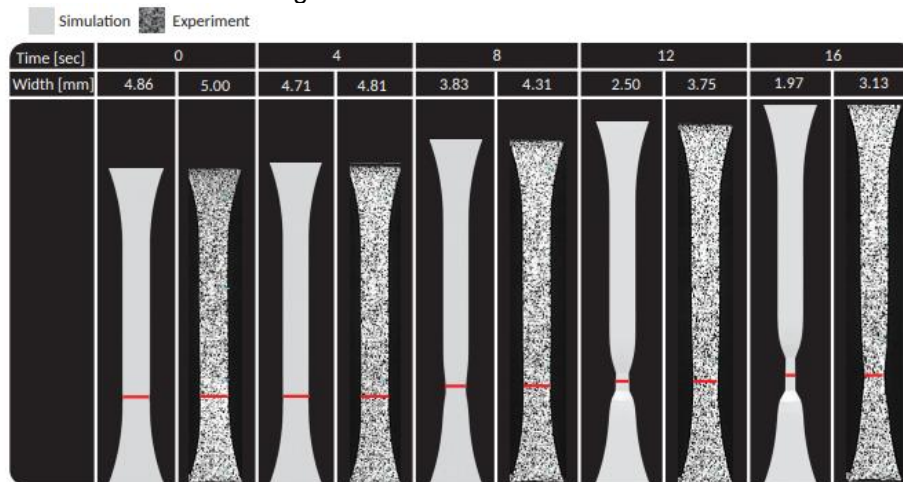


Fig. 4 Comparison of simulation and experimental deformation sequences [4]

The final test for the FFNN2 network was to check how well it can generalize to determined F-D of HDPE of different grades with different F-D response. For this purpose, several HDPE grades were tested on same geometry, and experimental F-D was fed to the trained network for hardening model prediction. The model predicted coefficients were given to the FE-solver Abaqus and the resulting F-D were plotted together with the experimental F-D as can be seen in Figure 6 showing very good FFNN2 performance. This makes it applicable for the intended use of determining the hardening values from tensile test F-D curves for various grades.

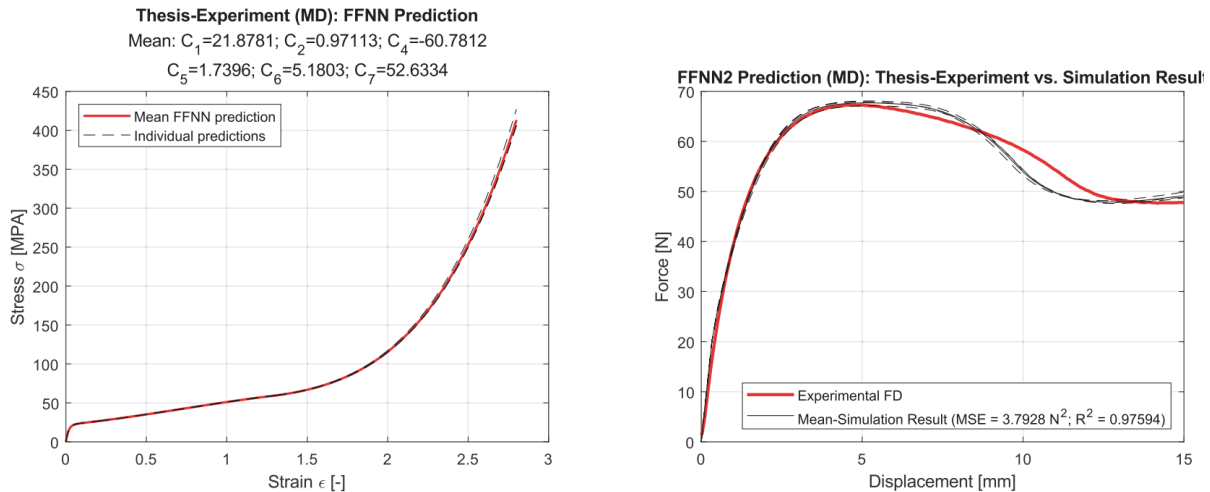


Fig. 5 FFNN: Prediction of hardening curve and experimental tensile test vs FE-response. [4]

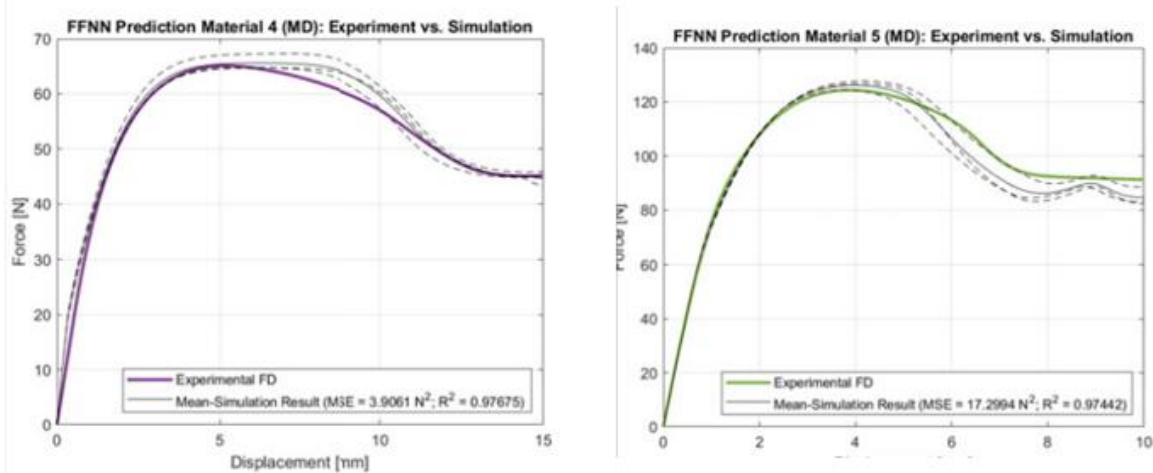


Fig. 6 Prediction accuracy of hardening curve on unseen experimental F-D. [4]

## 5 Conclusions

This study presents a new elasto-plastic hardening model for HDPE and a novel approach to the model calibration using artificial neural networks, specifically feedforward neural networks (FFNNs). The method improves efficiency and accuracy for proposed hardening model parameter calibration offering substantial benefits for the packaging industry. The prediction accuracy of the trained FFNN models on unseen HDPE grades demonstrated the proposed calibration method to be well generalized. This study provides a foundation for future research in applying machine learning techniques to material model calibration of similar polymers.

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# Modelling of Visco-Plasticity Using Neural Networks

Martin Kroon (Linnaeus University)

## 1 Summary

Neural networks can be used to replace complicated functional expressions. In the present work, neural networks are employed to model material hardening and rate-dependence of materials. The material model consists of an Eulerian framework (i.e. all state variables are defined in the current state of the material), and neural networks are added to this framework. The framework as such has been developed in previous works, and in the present work, neural networks are used to model the rate-dependence and hardening of the material. That is, no functional expression for these behaviours need to be defined in advance. The neural network-based model is applied to both theoretical reference data as well as actual experimental data in the form of stress–strain data. Different optimisation methods are explored for optimising/training the neural networks. The model was able to reproduce both the theoretical reference solutions as well as the experimental data very well. An implicit FE formulation is also provided in the form of a subroutine (UMAT) in Abaqus. The implementation was applied to two 3D examples, and the implementation seems to be robust and shows nice convergence properties. Overall, the present neural network-enhanced framework seems to be promising and there is potential for further development.

## 2 Theoretical framework

The constitutive model is Eulerian in the sense that all state variables are defined in the current state of the material. In the following presentation, standard notation is used, and all variables are therefore not explained explicitly. The elastic deformation state of the material is defined by use of the two state variables  $\bar{\mathbf{B}}_e$  and  $J$ , where  $\bar{\mathbf{B}}_e$  is the unimodular version of the elastic left Cauchy-Green deformation tensor, and  $J$  is the elastic dilatation. These two state variables evolve according to

$$\dot{\bar{\mathbf{B}}}_e = \mathbf{L}\bar{\mathbf{B}}_e + \bar{\mathbf{B}}_e\mathbf{L}^T - \frac{2}{3}(\mathbf{D} : \mathbf{I})\bar{\mathbf{B}}_e - \Gamma\bar{\mathbf{A}}_p,$$

and

$$\dot{J} = J\mathbf{D} : \mathbf{I}.$$

Above,  $\mathbf{L}$  is the velocity gradient,  $\mathbf{D}$  is the rate of deformation tensor,  $\mathbf{I}$  is the identity tensor,  $\Gamma$  is a variable that determines the magnitude of inelastic/plastic deformations, and

$$\bar{\mathbf{A}}_p = \bar{\mathbf{B}}_e - \left( \frac{3}{\bar{\mathbf{B}}_e^{-1} : \mathbf{I}} \right) \mathbf{I}$$

The Cauchy stress is given by

$$\mathbf{T} = \frac{\rho}{\rho_0} \left( \mu \bar{\mathbf{B}}_e' + K(J-1)J\mathbf{I} \right) = \frac{\mu}{J} \bar{\mathbf{B}}_e' + K(J-1)\mathbf{I}.$$

Above,  $x'$  is the deviatoric part of  $x$ .

The yield behaviour of the material is described in strain space (rather than stress space which is more common), and a yield function,  $g$ , is introduced:

$$g = \gamma_e - (1 + \beta U)\kappa$$

Here,  $\gamma_e$  is an equivalent elastic strain (corresponding to the von Mises stress in stress-based formulations),  $\kappa$  and  $\beta$  are hardening parameters, and  $U$  is the Lode parameter, given by

$$U = \frac{27\det(\mathbf{T}')}{2\sigma_e^3} = \frac{27\det(\bar{\mathbf{B}}_e')}{16\gamma_e^3}$$

The magnitude of inelastic deformations,  $\Gamma$ , is expressed as

$$\Gamma = \left( \exp(\hat{b})\dot{\epsilon} + \hat{a} \right) \langle g \rangle,$$

where the parameters  $\hat{a}$  and  $\hat{b}$  are output from a neural network, and  $\varepsilon$  is an equivalent measure of distortional deformation rate. Furthermore, the evolution of the hardening variables is given by

$$\dot{\kappa} = \Gamma \hat{\kappa},$$

and

$$\dot{\beta} = \Gamma \hat{\beta},$$

where  $\hat{\kappa}$  and  $\hat{\beta}$  are two additional parameters that stem from a neural network. The use of the neural network can be illustrated as in Fig. 1.

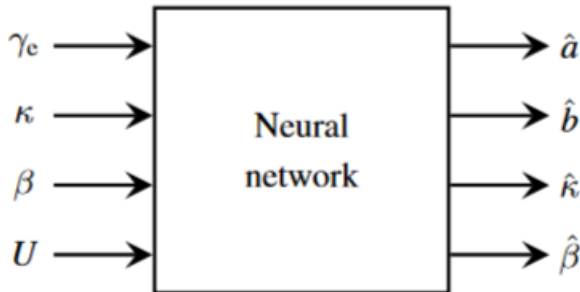


Fig. 1. Illustration of neural network with input and output variables.

### 3 Results and Discussion

Simple feed-forward neural networks are used in the present study, and in most cases a single hidden layer is used ( $n_h = 1$ ). The number of neurons ( $n_w$ ) in this layer is varied. Poisson's ratio is assumed to be  $\nu = 0.3$  or  $0.4$  depending on which material is considered (steel or polymer). The shear modulus is estimated during the training procedure. The error function,  $l$ , is defined as the average mean square difference between the reference stress response and the trained stress response. In the graphs below,  $i_e$  denotes the number of epochs in the training procedure.

In the first example, the neural network is trained by use of a theoretical reference curve. In this case, rate-independent material response is considered. The outcome is shown in Fig. 2.

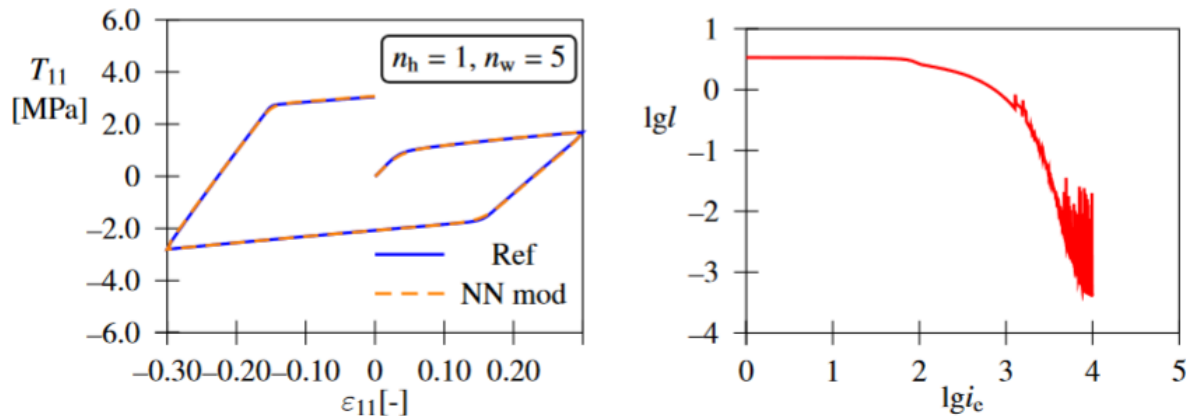


Fig. 2. Training of neural network model by use of rate-independent reference stress data. (a) Reference and trained stress response. (b) Evolution of error function  $l$  during the training process.

The neural network model is able to reproduce the reference curve almost perfectly. In this case, 5 neurons were used in the hidden layer in the neural network. Fig. 2(b) shows the evolution of the loss function. As can be seen, it takes about 10000 iterations in the training loop before a really good fit has been accomplished.

Fig. 3 shows the outcome when the neural network model is applied to stress data where the uniaxial test is simulated at three different strain rates. Hence, in this case we have a rate-dependent response of the material. The neural network model is able to model these data almost perfectly as well. Again, it takes about 10000 iterations in the training loop to obtain a really nice fit of the neural network model, as seen in Fig. 3(b).

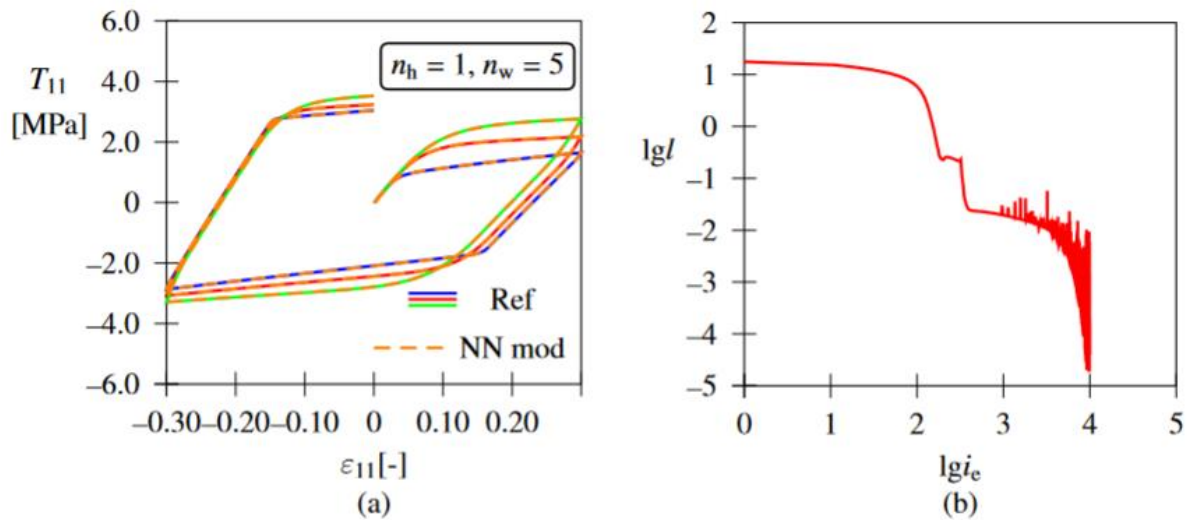


Fig. 3. Training of neural network model by use of rate-dependent reference stress data. (a) Reference and trained stress response. (b) Evolution of error function  $l$  during the training process.

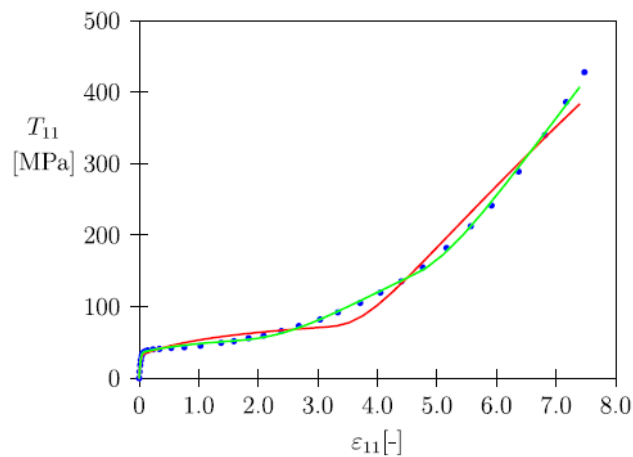


Fig 4. Neural network representation of material hardening in HDPE [1]. Experiments (symbols) and neural network model with  $n_w = 3$  (red line) and  $n_w = 5$  (green line).

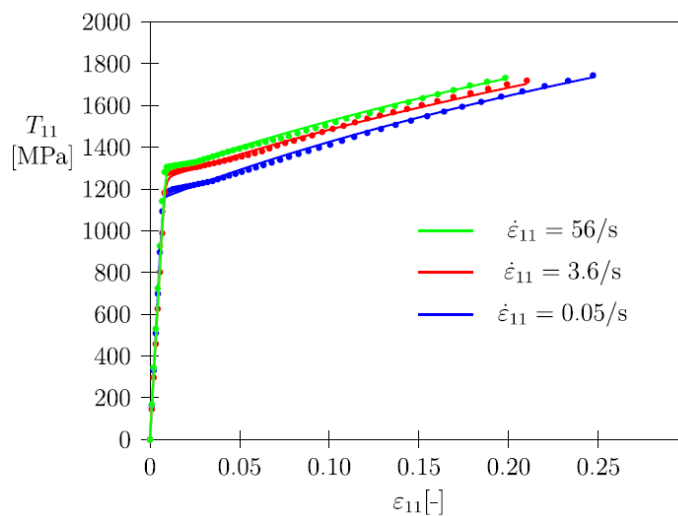


Fig. 5. Neural network representation of material hardening and rate-dependence of high-strength steel [2].

The neural network model is also applied to real experimental data. The first set of data is from testing of polyethylene [1]. Fig. 4 shows the experimental values from a uniaxial tensile test performed up to strain levels approaching 800%. In the neural network model, a hidden layer with 3 and 5 neurons was

explored. The model with 3 neurons produces a representation that is relatively crude. But with 5 neurons, a relatively smooth representation of the experimental results can be accomplished.

Finally, the neural network model is applied to experimental data performed on a high-strength steel at different strain rates [2]. The outcome of the training procedure is shown in Fig. 5. The model is able to represent the hardening (which is close to linear) and also the strain-rate dependence of the hardening.

More details about the present neural network model can be found in the journal paper [3].

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# AI-Driven Design Parameter Optimization for Sheet Metal Forming Processes

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## 1 Summary

We present an AI-based approach for optimizing sheet metal forming processes like deep drawing. Given the desired shape of the deformed metal sheet, our methodology varies process parameters such as the applied forces and the initial thickness of the undeformed sheet to optimize objective functions like the maximum thinning and thickening of the sheet or the amount of wrinkling. Our workflow comprises four main components: a deep neural network, a finite-element simulation software system, a decision component, and a Bayesian optimization or active-learning routine. The deep neural network is pre-trained and used to generate a set of possible initial process parameter vectors for the given geometry. Next, we perform a finite-element simulation to check whether any initial value vectors yield a sufficiently good result. If this is not the case, the decision component considers the user's requirements, the precise objective function, the given data, and the available resources. Based on this information, it selects whether to proceed with the parameter optimization process via Bayesian optimization or active learning.

## 2 Introduction and Formulation of the Problem

In many engineering processes, it is necessary to produce metal sheets with complex geometric shapes. Classical examples for such a problem are the manufacturing of car body parts in the automotive industry or the production of components for household appliances. One of the most common techniques to achieve this goal is the deep drawing method [4] where an initially plane sheet of metal is drawn into an appropriately shaped die by the mechanical action of a punch.

Classical simulation codes for sheet metal forming processes are established and well-understood tools for solving the associated forward problem of determining the shape and many other properties of the workpiece under the assumption that the process parameters (forces, tool geometries, material properties etc.) are given. Consequently, this obviates the need to create one or more prototype(s). The task of the domain expert working with such tools can be described as the corresponding inverse problem: Given the target shape of the object, its required main properties, and minimum quality standards, they need to find suitable process parameters that lead to the desired result.

The number of involved parameters that can be tuned to optimize the deep drawing process is relatively large, and the influence of a change in any of these values on the final result of the deep drawing process is often very difficult to predict. Therefore, even an experienced process planning engineer requires many iterations and thus a substantial amount of time to find an acceptable set of parameters. This is where we aim to contribute by providing an AI-based approach that automates several steps in this optimization task, thus supporting the engineer in their search of such process parameter sets while simultaneously reducing the required number of working hours.

## 3 Description of Our AI-Driven Approach

Our approach consists of several interconnected components as shown in the schematic visualization given in Figure 1.

The first component of the workflow is a deep neural network (DNN). The user, typically a domain expert in deep drawing, provides information for this network regarding the target geometry, the material properties of the metal sheet, and the admissible ranges of the process parameters that may be tuned (e.g., the blank thickness, the forces to be applied by the tools, friction coefficients, and many

more). The DNN is pre-trained using a large set of simulation data from known metal forming processes. Based on the training data, it generates an initial parameter set for the process currently under consideration and estimates the properties of the resulting workpiece. If the domain expert believes that this outcome is acceptable then we include these parameters into the input deck of our sheet metal forming simulation code OF/Solv – the finite element based solver component of the OpenForm sheet metal forming simulation software package [2] – and simulate the process in order to validate the result. After a successful validation, the production process for the workpiece can be started with the process parameters that the DNN has found, so that the problem has been solved and the task is completed.

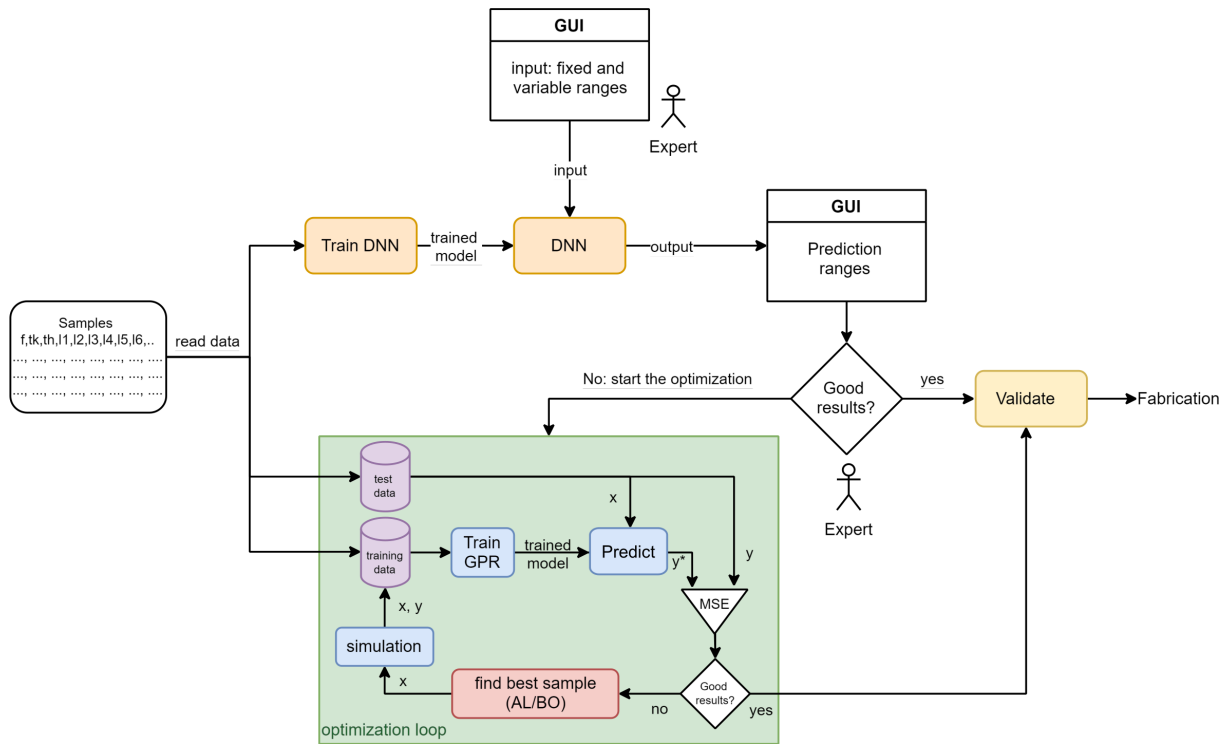


Fig. 1 Schematic visualization of our AI-assisted workflow for design parameter optimization in sheet metal forming to reduce the involvement of the domain expert by, among others, a DNN and Bayesian optimization

Otherwise, if the DNN’s proposed parameter set is not yet sufficient to match the demands, our workflow enters the optimization cycle indicated in the green box in Figure 1. In this step of the process, we run through a Bayesian optimization loop to improve the process parameter values until we reach a satisfactory state. Given the very limited knowledge of the characteristics of the target function, we use a derivative-free black-box optimization scheme [3] here. The required sampling strategies are based on the concept of acquisition functions [1] where, specifically, our code may use a Gauss process upper confidence bound, the probability of improvements, or the expected improvement. One of the outcomes of our experiments with these acquisition functions (see Section 4) is that typically the number of iterations required in the optimization cycle is relatively high when the probability of improvements is used as the acquisition function and much smaller for the two other choices.

A particularly noticeable fact about this optimization loop is that it runs in a fully automatic manner. No intervention or input by the human expert is required. Once the results are good enough, we validate them using an additional simulation, and the task is completed.

To improve the system’s performance, we re-train the DNN used in the initial process step after each successful program run by adding information about the obtained satisfactory solution.

## 4 Results

As an example, we have used the process of deep drawing of a cylindrical cup as shown in the left part of Figure 2. This is a standard test case in sheet metal forming. The image shows the results of a

forming simulation using the OF/Solv software system. It specifically visualizes the main component of the target function that we have chosen in this example, namely the so-called formability of the workpiece. To evaluate this criterion, the simulation system computes the material thinning and the stresses and strains at each element of the workpiece's finite element discretization. The formability is then classified locally according to the obtained results either as being safely feasible (shown in green in the figure) or as belonging into one of six undesired categories (insufficient stretch: gray, severe wrinkling: purple, wrinkling tendency: blue, severe thinning: orange, risk of cracks: yellow, or cracks: red). The process planner's goal, and hence our objective function in this case, is to maximize the size of the region that is classified as safe.

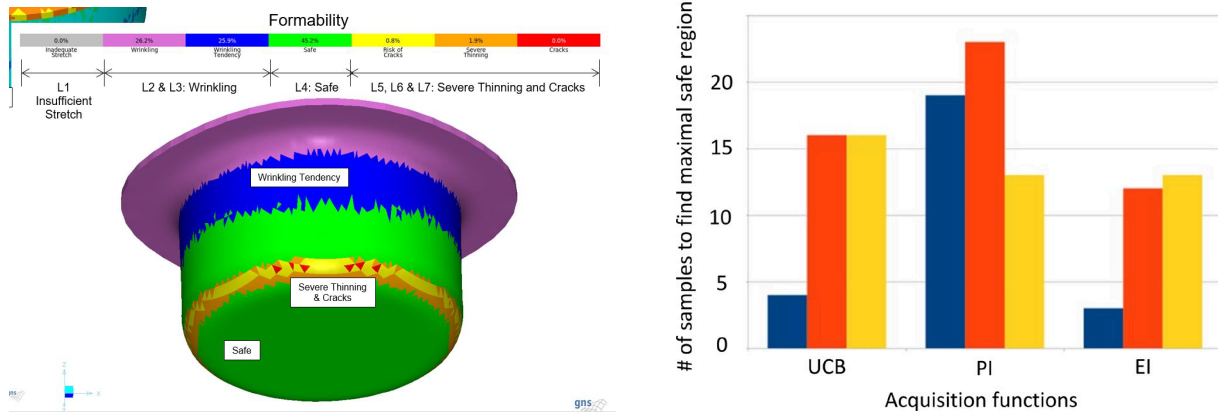


Fig. 2 Left: Forming feasibility results for cylindrical cup, obtained by a simulation using the OpenForm FE solver OF/Solv and visualized in its postprocessor OF/Post. Right: Required number of iterations to maximize the safe region's size when using different acquisition functions. The blue bars refer to situations where the initial guess was close to the optimal solution, for the yellow bars it was far away, and the red bars correspond to an intermediate distance.

The right part of Figure 2 shows the performance of our Bayesian optimization loop. As one may have expected, the number of iterations depends on the chosen acquisition function and the quality of the initial guess for the process parameter set. But it is also evident that, for the expected improvement (EI) and upper confidence bound (UCB) acquisition functions, the process converged to the optimum in a relatively small number of iterations.

## 5 Conclusions

The optimization of deep drawing processes in sheet metal forming is a challenging task that so far has required a substantial amount of manual effort by human experts. Our newly developed and implemented AI-based methodology allows to automatize this optimization process to a significant extent. The test cases which we have discussed so far indicate that the approach yields very satisfactory results with a major reduction of the necessary human interaction.

## 6 Acknowledgement

The work described in this talk is supported by the German Federal Ministry of Education and Research (BMBF) under Grant No. 16ME0631.

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# Applications of AI in Engineering

Gustaf Jönsson (Application Engineer)

## 1 Summary

This summary outlines three innovative simulation cases using reduced-order modeling (ROM) and Geometric Deep Learning (GDL) to enhance efficiency in industrial processes and engineering design.

1. **Drivetrain CFD Simulations with ROM:** A ROM approach was used to predict thermal behavior in a gearbox, leveraging data from high-fidelity fluid simulations to estimate heat transfer coefficients. This ROM enabled rapid, accurate predictions in a system-level thermal model, achieving over 130,000 times speedup compared to full-scale simulations. This method holds potential for applications requiring quick, dynamic predictions in design and optimization.
2. **Bulk Solids Handling Optimization with ROM:** This project introduced a virtual optimization framework for industrial bulk handling, combining simulations with ROM and machine learning to reduce computational costs. The ROM provided a link between process parameters and key performance indicators, allowing efficient identification of optimal conditions. This framework could be extended to other industrial processes, supporting faster and more informed operational decision-making.
3. **Radar Cross Section (RCS) Predictions with GDL:** Geometric Deep Learning (GDL) was applied to predict RCS for various aircraft designs. By training on a dataset of high-fidelity simulations, the GDL model offered accurate predictions even on new designs, greatly reducing development time. This approach has potential for a range of complex physics-based problems, enabling efficient design and evaluation in fields such as aerospace and defense.

Each case illustrates the value of integrating ROM or GDL in simulations, showcasing how these methods enable rapid, resource-efficient predictions for complex systems.

## 2 Reduced Order Models (ROMS)

### 2.1 Using rom with Drivetrain CFD simulations

Using ROMS can help to efficiently predict the thermal behavior of gearboxes during operations by reusing data from smooth particle hydrodynamics (SPH) oil flow simulations, see figure 1.

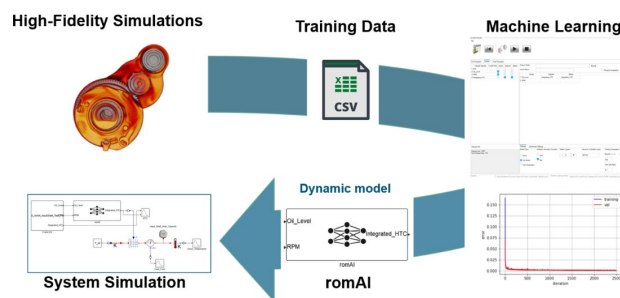


Fig. 1 – Overview of methodology used to predict thermal behavior of gearbox with system simulations and ROM.

In this project, by utilizing the results from multiple nanoFluidX oil flow simulations, a ROM was generated that estimates the heat transfer coefficient (HTC) between the oil and the structural components as a function of RPM & Oil fill level, see figure 2. Altair's romAI was used to generate the ROM in this case. 5 different simulation were used as the training data for the ROM.



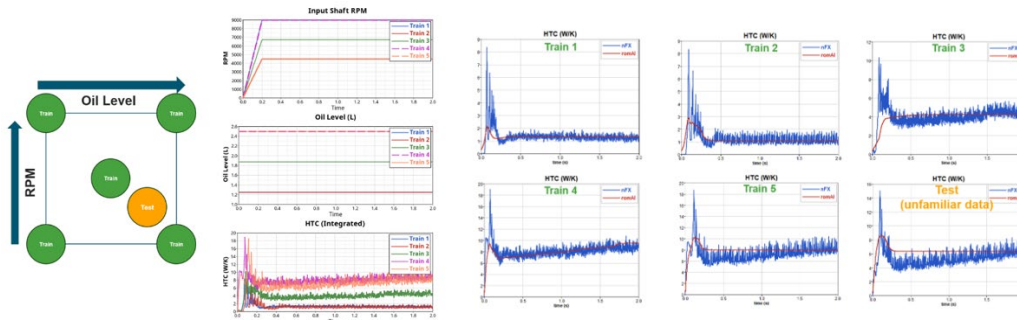


Fig. 2 – Data of HTC obtained from SPH simulation (left) and the prediction behavior of the trained ROM (right).

This ROM is then used as an input into a 1D lumped parameter thermal model represented in a system level simulation model. The thermal model consists of “heat exchanger” and a “heat capacitor” blocks that are used in combination with sensors to measure the average temperature of components and heat flow, see figure 3.

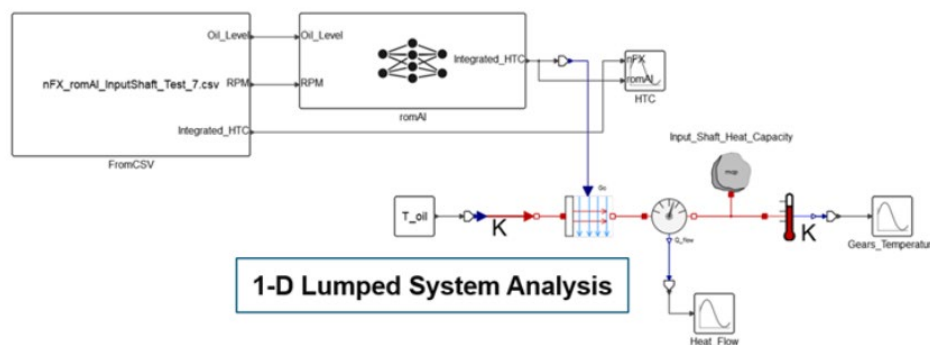


Fig. 3 – System simulation model of drive train with ROM-block included.

The model can give a good indication of the heat transferred, especially considering that the HTC integrated over the area of components is estimated accurately from high-fidelity simulations. By running the combined system simulation on the unfamiliar test case, it's possible to get the results for the heat flow and gear temperature as a function of time, see figure 4.

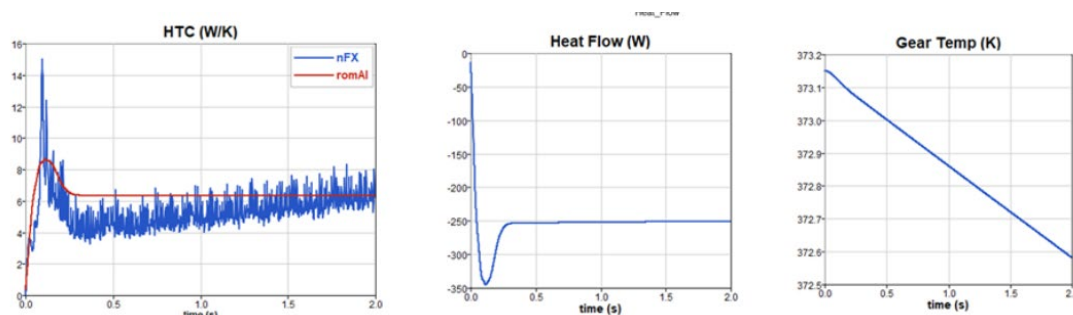


Fig. 4 – Results from the system simulation using ROM.

By utilizing this methodology, we can see that relatively few SPH simulations are needed to train a ROM that is able to make dynamic predictions with high accuracy. The speedup of using the ROM versus the full SPH simulation is more than 130.000 for this case, which enables the possibility to do vast 1-D DOE studies and optimization in a short period of time.

## 2.2 Using rom with simulation for efficient bulk solids handling optimization

In this project, we present an efficient virtual optimization methodology for industrial bulk handling processes, which combines high-fidelity numerical modelling in EDEM with statistical and machine learning methods to significantly reduce the computational expense of optimization relative to a purely simulation driven approach. The proposed methodology is conceptualized in Figure 5.

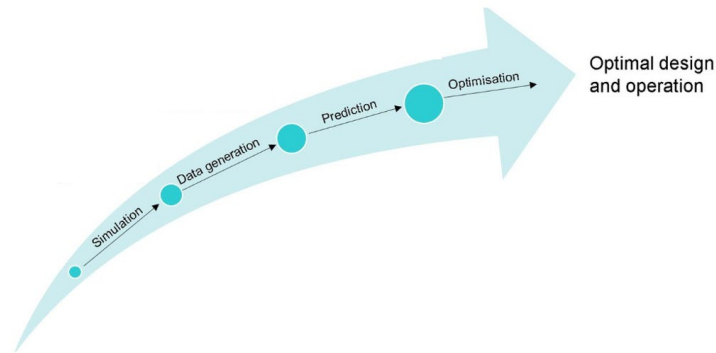


Fig.5 – Methodology for efficient virtual optimization for industrial bulk handling process.

Altair HyperStudy is employed for the automatic generation of a statistically efficient dataset of EDEM simulations and the machine learning algorithms in romAI are leveraged for the generation of a dynamic ROM of the system, which relates process operational parameters to Key Performance Indicators (KPIs). An optimization algorithm in Altair Activate is then used to operate on the reduced-order model to rapidly identify the optimal operational parameter values.

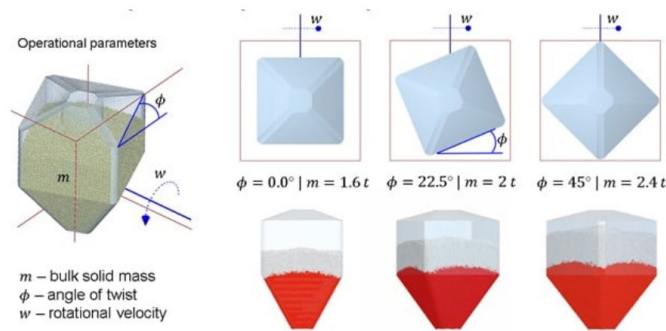


Fig.6 - Blender operational parameter space.

In this case, the blender operational parameters include the rotational velocity, the angle of twist and the mass in the system, as described in Figure 6. The KPI of interest is the time evolution of the mixture uniformity as quantified by the Segregation Index in Equation 1, where  $C_{ij}$  is the number of contacts between particle types  $i$  and  $j$ .

$$SI = \sum_{i,j} \left( \frac{C_{ii}}{\sum_j C_{ij}} \right) \quad (1)$$

The segregation index is inversely proportional to mixture uniformity and should decrease with mixing time, see figure 7.

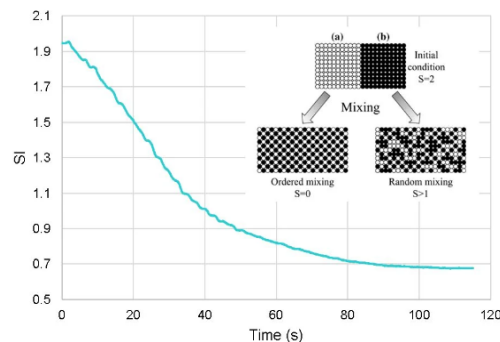


Fig.7 - Example result for the time evolution of the Segregation Index in an EDEM bin blender model.

HyperStudy's Design of Experiments (DoE) feature is used to generate and run a data set of EDEM simulations according to a three factor - three level Taguchi design.

### 2.3 Reduced order modelling

In the context of this work the ROM is conceptually illustrated in Figure 8 and takes the blender operational parameters as inputs and the segregation index as output.

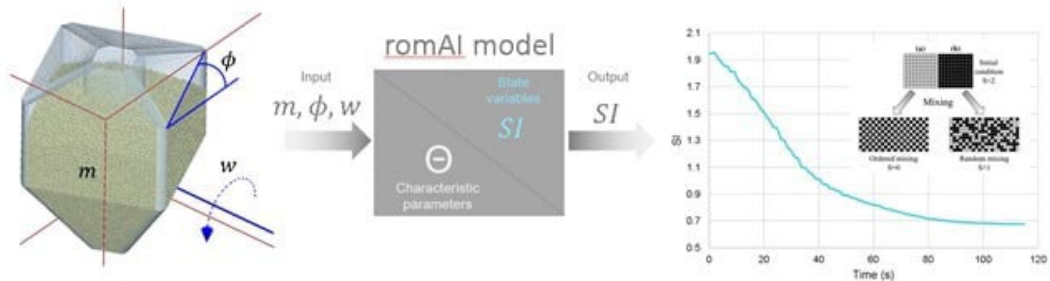


Fig.8 - A conceptual representation of the romAI dynamic model developed in this work.

### 2.4 Parameter optimization

We connect our ROM model to the system simulation software Activate's gradient descent based optimizer in order to rapidly identify the optimal blender operational parameter set.

The model prediction for the optimal parameter set is verified against the EDEM simulation results and an excellent agreement can be observed as shown in Figure 9, demonstrating the validity of the approach.

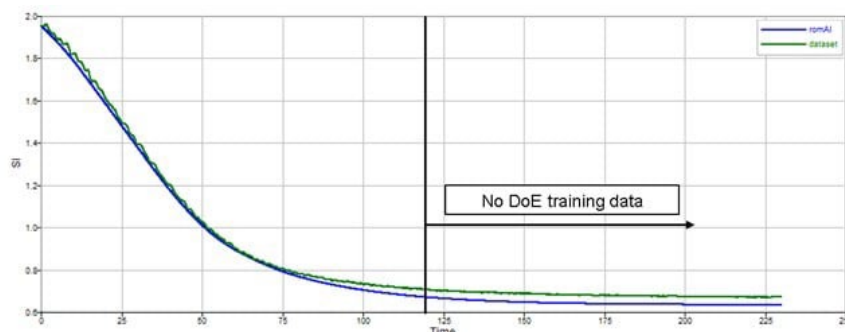


Fig.9 - Verification of the optimal parameter set - romAI prediction vs EDEM simulation result.

## 3 Geometric deep learning (GDL)

Geometric Deep Learning is a field of machine learning focused on applying deep learning to non-Euclidean data structures, like graphs, manifolds, and other complex geometries. Unlike traditional deep learning, which typically operates on regular grids (e.g., images or sequences), geometric deep learning methods can capture the intricate relationships and structures present in spatial, relational, or irregular data. This field enables applications across domains such as social networks, 3D objects recognition, biology, and physics, where data is naturally represented by these more complex forms.

### 3.1 Radar Cross Section (RCS) predictions with GDL

Radar Cross Section (RCS) is a measure of how detectable an object, like an aircraft, is by radar. It represents the area that reflects radar signals back to the source and is influenced by the size, shape, materials, and angle of the aircraft relative to the radar. RCS is crucial in designing military aircraft and stealth technology, where the goal is to minimize detectability by reducing RCS through materials that absorb radar waves, shaping surfaces to deflect radar, and incorporating features that scatter radar energy. Reducing RCS enhances an aircraft's ability to evade detection, which is vital in both offensive and defensive military operations. Using GDL for prediction of RCS for different geometrical designs can greatly speed up the design process.

For this case, 146 FEKO simulations with different aircraft designs were generated with design variables and output responses according to figure 10.

- Create RCS result data (@ f = 350 MHz) for different wing shapes

• **4 design variables:**

- DH: Change height of profile
- DX: Change length of wing
- DY: Change width of wing
- DZ: Change slope of wing

• **Response:**

- Monostatic RCS for  $\theta = 0^\circ, \dots, 180^\circ$  at  $\phi = 0^\circ$
- 2 Polarizations:  $\eta = \{0^\circ, 90^\circ\}$

	Active	Label	Varname	Lower Bound	Nominal	Upper Bound
1	<input checked="" type="checkbox"/>	DH	var_1	0.1000000	0.1500000	0.2000000
2	<input checked="" type="checkbox"/>	DX	var_2	0.0000000	1.0000000	4.0000000
3	<input checked="" type="checkbox"/>	DY	var_3	0.7650000	0.8500000	1.2000000
4	<input checked="" type="checkbox"/>	DZ	var_4	0.0000000	0.1000000	0.1000000

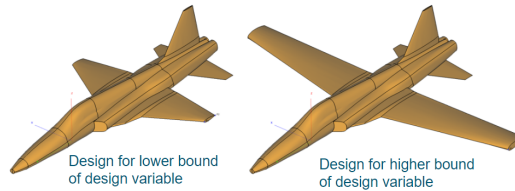


Fig.10 - Design variables and responses generated by FEKO DoE.

The simulation results are then used to train a GDL model with the use of physicsAI in HyperMesh. The dataset is split up into a training dataset and test dataset to be used for training and testing of the model respectively. The resulting Mean Absolute Error (MAE) score of the model is given in figure 11 below.

- **Training Dataset:** 131 files
- **Test Dataset:** 15 files
- **Hyperparameter:**
- **Walltime:** 01:52:06
- **Memory requirements:** 2.88 GB

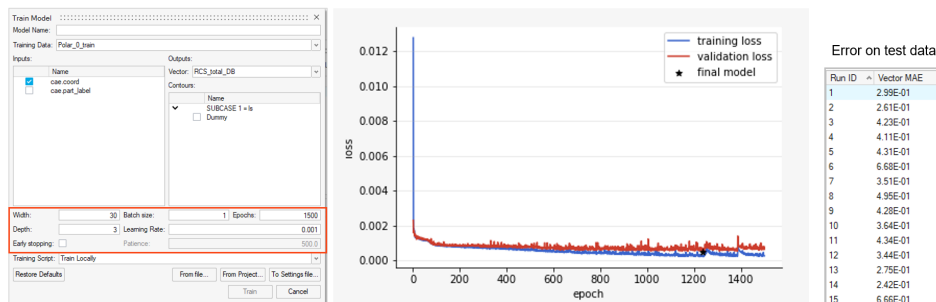


Fig.11 - Overview of training/validation loss and MAE for GDL model for RCS prediction.

Performing a validation of the GDL on geometrical designs that is has not been trained on, we can see that its able to capture the monostatic RCS with high accuracy, see figure 12.

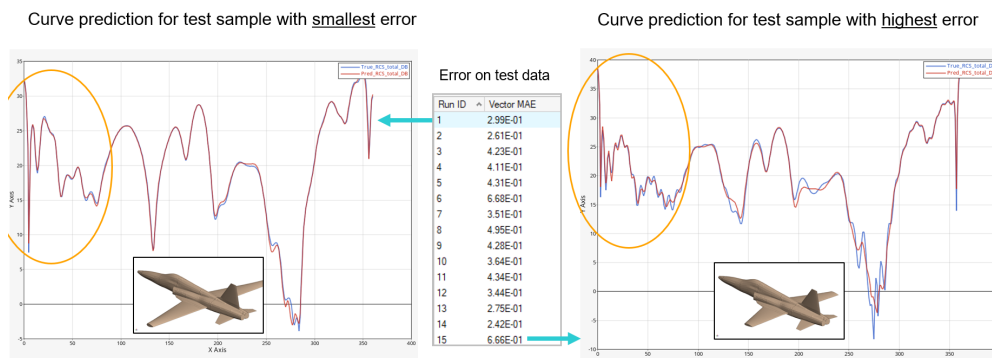


Fig.12 – Results of GDL prediction on unseen geometrical design of the aircraft.

By utilizing a GDL simulation based approach, its possible to achive significant reduction in model build time and prediction time of the type of physics the GDL model has been trained on. This adds value by reducing development time and making it possible to make design decisions faster.

## **4 Conclusions**

### **4.1 Using rom with Drivetrain CFD simulations**

This project demonstrates the effectiveness of a ROM approach for predicting thermal behavior for gearbox heat transfer analysis. By reusing high-fidelity simulation data, the ROM accurately captures heat transfer dynamics based RPM and oil fill levels. The integration of the ROM into a system-level thermal model enables rapid predictions with minimal computational resources, achieving a speedup of over 130,000 times compared to full-scale simulations. This methodology shows potential not only for drivetrain analysis but also for broader applications where efficient, dynamic predictions are essential, supporting large-scale design exploration and optimization.

### **4.2 Using rom with simulation for efficient bulk solids handling optimization**

This project presents an efficient virtual optimization methodology for industrial bulk handling processes by combining high-fidelity simulations with reduced-order modeling and machine learning. This integrated approach significantly reduces computational costs compared to traditional, simulation-driven methods, enabling rapid identification of optimal process parameters. By validating the model's predictions against full simulations, the methodology proves to be both accurate and efficient. This framework also highlights the potential for applying similar optimization techniques across other complex industrial processes, ultimately enhancing decision-making and operational efficiency.

### **4.3 RCS predictions with GDL**

Using GDL for RCS prediction offers significant advantages in speeding up design and evaluation processes. This approach not only reduces reliance on time-intensive simulations but also provides accurate predictions on new designs, enabling faster and more efficient design decisions. The success of GDL in RCS prediction highlights its potential for other physics-based problems and complex geometries, making it a valuable tool for various engineering and scientific applications where rapid, reliable predictions are essential.

# Combining Simulation with Machine Learning During Various Design Phases of Turbomachinery.

Erik Munktell, (Siemens); Gabriel Amine-Eddine, (Siemens); Rene Braun, (Siemens);

Justin Hodges, (Siemens); Stephane Mouvand, (Siemens)

## 1 Summary

Figure 1 shows the “classical” approach of a CAD image from a jet engine assembly using NX. Designing a gas turbine in the past would take several years and would not always be a success. Thanks to digital tools, we can improve on today’s design quite easily with a multidisciplinary approach of design an optimization.

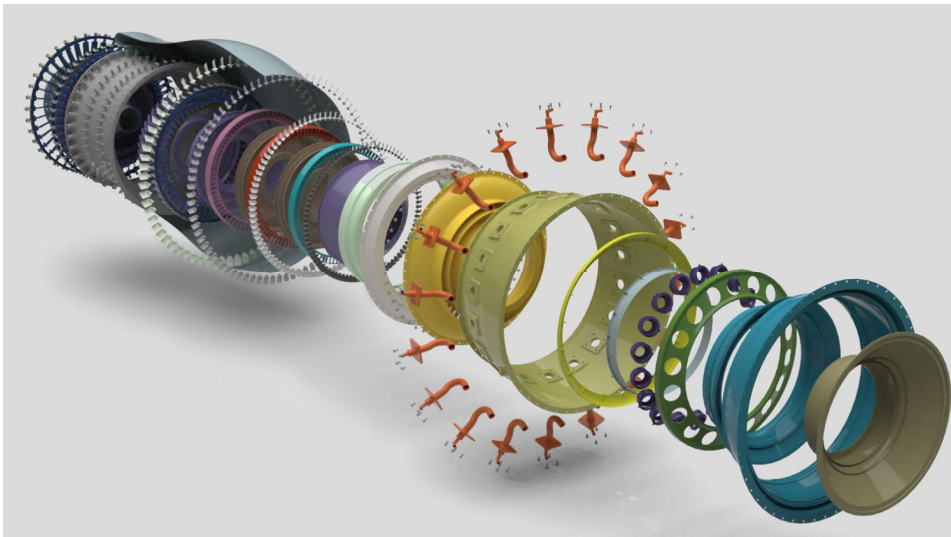


Figure 1: Jet engine assembly (Generated with NX).

Even though it is very advanced physics and complex geometries, one can today combine several of these steps in an automated way. Keeping the CAD alive, boundary conditions and various versions stay totally in your control. The design process of a component is shown in the schematic of Figure 2. This is done by joining the CAD from NX to various CAE simulation tools like Simcenter STAR-CCM+ and Simcenter 3D. The automation and optimization are handled by HEEDS and all data is managed by Teamcenter.

It really does not matter if it is higher efficiency through aerodynamics, improved mechanical integrity and durability, reducing cooling air usage or new combustion fuels; they all affect each other and there is no way to be competitive and innovative unless correctly using modern multidisciplinary design space exploration methods. To effectively do product development, we want to evaluate as many designs as early on in the process as possible. Taking the next steps into the future means combining this with machine learning, since the design space can become large quickly and with many disciplines involved.

## 2 Chapter

In order to effectively do product development, we want to evaluate as many designs as early on in the process as possible. Taking the next steps into the future means combining this with machine learning, since the design space can become large quickly and with many disciplines involved. What if we could have a machine learning algorithm train itself in real time on the design space that is currently being evaluated with computational fluid dynamics (CFD) or finite element method (FEM)?

For that, we have a few proofs of concept that are related to turbomachinery. One example is to optimize a water pump efficiency at a flow rate of 110 kg/s and 1200 rpm. We worked on a parametrized model with 12 geometric variables and the number of blades.

HEEDS, a multi-disciplinary design analysis and optimization (MDO) software, uses its default search method, SHERPA, to conduct multiple search strategies simultaneously, and it dynamically adapts to the problem as it learns about the design space. In the standard setup we ran 300 design variations in 40 hours. With the introduction of HEEDS AI Simulation Predictor, [1] SHERPA's search technology is significantly enhanced. Some CFD simulations are replaced by AI evaluations conducted through an automatically trained AI model, leveraging insights gained from early simulations – revolutionizing this process. In this case, it counted 151 CFD runs while 149 were done with AI evaluation (for a total of 300). This took roughly 20 hours reaching the same results and saving 49% in time. The pump's efficiency increased by 3% and head by 10%.

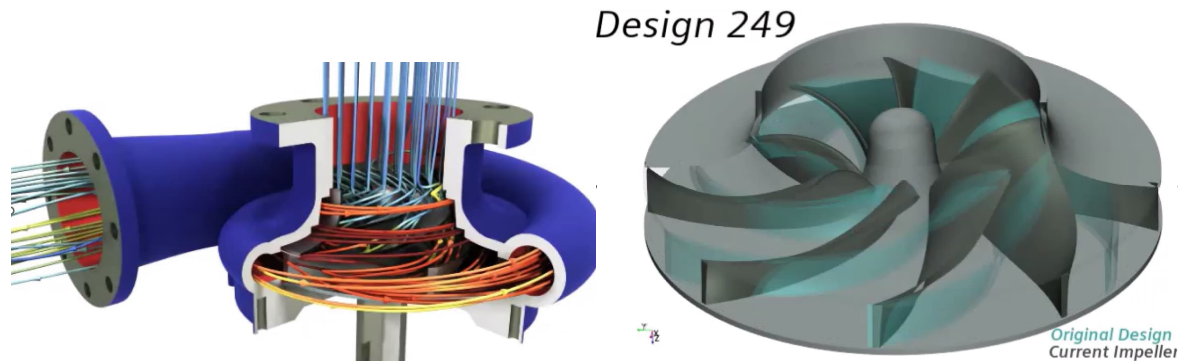


Figure 3: Water pump - design space exploration with HEEDS AI Simulation Predictor - CAD and CFD results

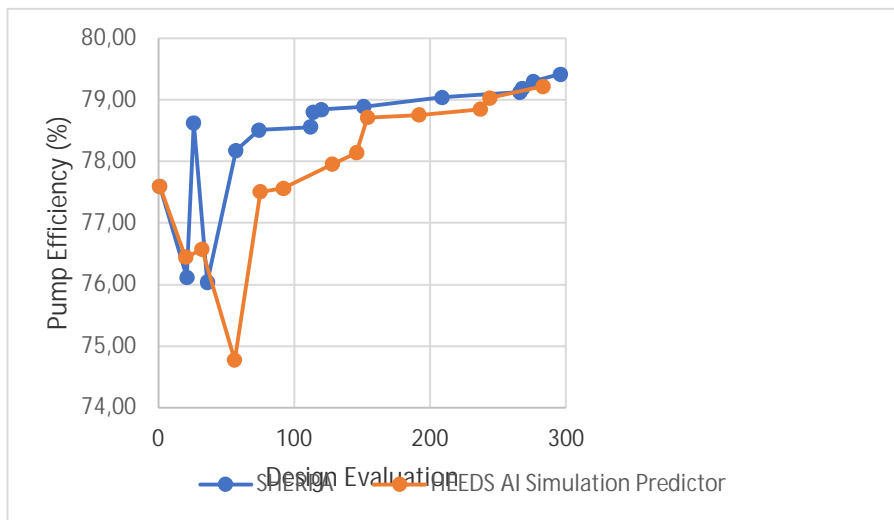


Figure 4: Water pump efficiency for various designs - design space exploration with HEEDS AI Simulation Predictor.

The second case is a gas turbine blade for cooling optimization. Here, the objective is to minimize blade temperature and minimize cooling air mass flow. A parametrized CAD from NX is used to simulate in Simcenter STAR-CCM+. The CAD has 34 parametrized characteristics on the serpentine channel with changes of cooling ribs and shower head holes (see Figure 6). The 500 design evaluations done for this case experienced an approximate 38% time save, skipping CFD simulations with AI and still reaching the same best solution.

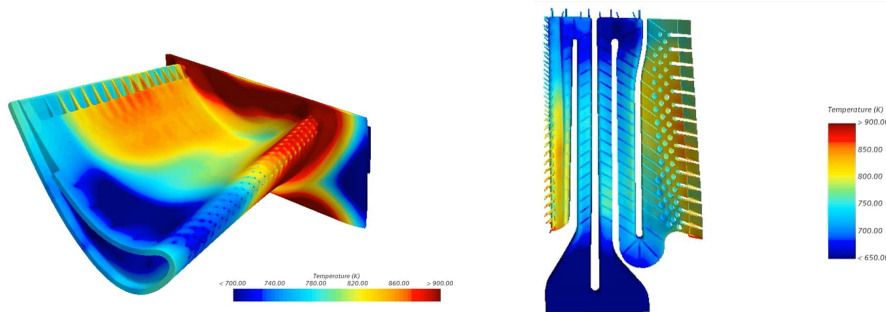


Figure 5: External and internal temperature for conjugate heat transfer turbine blade design space exploration with HEEDS AI Simulation Predictor, NX and Simcenter STAR-CCM+ .

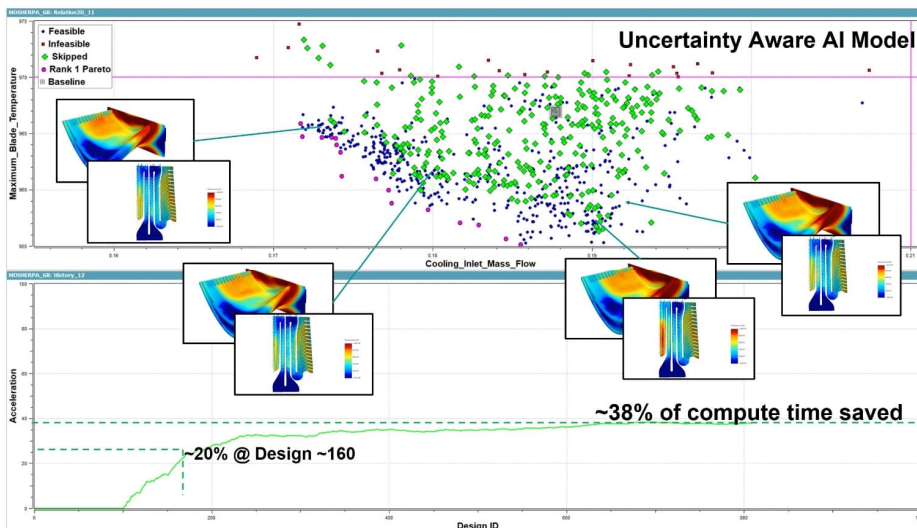


Figure 6: Pareto front of design space exploration for minimizing blade temperature and reducing cooling inlet mass flow results using HEEDS AI Simulation Predictor.



Reduced order models sometimes also uses machine learning and neural networks to enable data driven faster models. We have run a systems simulation model on a gas turbine and CFD of a heat exchanger in order to do real time simulations and use simulations in operations of the equipment. I will also show a few examples done by Siemens Energy and others in the turbomachinery industry and how they use machine learning to further speed up simulations [2], [3].

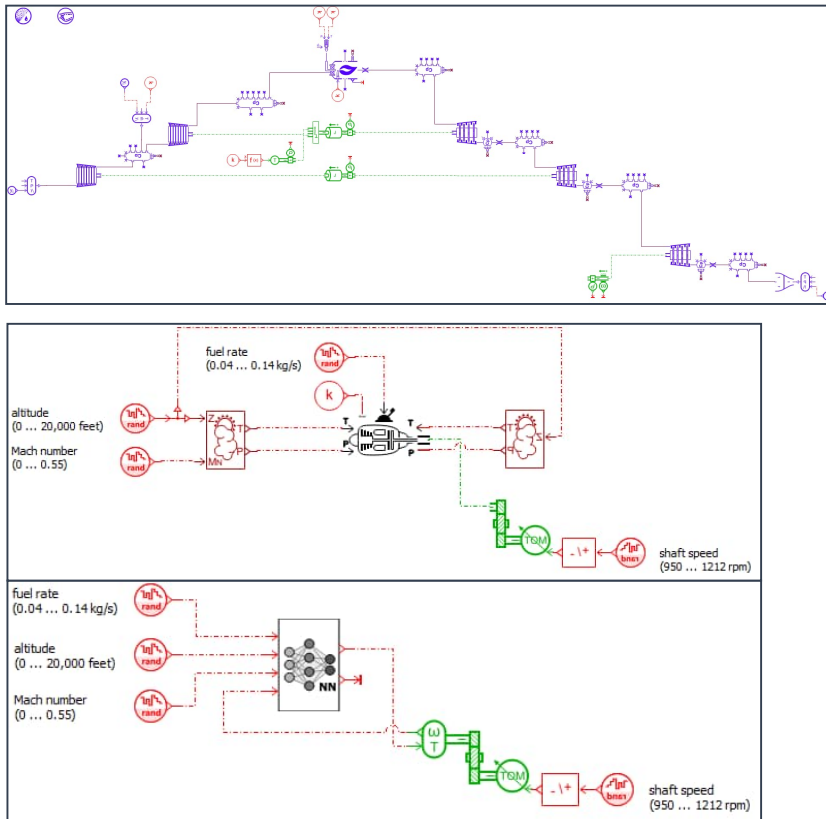


Figure 6: Real time simulations of a gas turbine system trained using neural networks.

### 3 Conclusions

From these first examples of adding AI and machine learning to an already impressive CAD-CAE workflow, one can already see the potential of machine learning for the turbomachinery industry. How big the revolution of AI and ML will be and the impact it will have on the fate of the mechanical industry is too early to say. But we already know that it will be the key to staying in front of the competition.

### 4 References

- [1] [Decomposition of uncertainty in Bayesian deep learning for efficient and risk-sensitive learning](#)  
S Depeweg, et al. 2018
- [2] [Surrogate](#) models for 3d Finite element creep analysis Acceleration  
J Abdallah, et al. 2023
- [3] A Real-Time AI-based Strategy For The Design Of A Low-Pressure Turbine Profile, GT2024-128809, Bellucci et al.

# Data-driven optimization of exhaust valve geometry for wear reduction

Mohammad A. Haghnejat (Wärtsilä / FS Dynamics),

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Niclas Liljeldfeld (Wärtsilä),

Luc St-Pierre (Aalto University)

A well-engineered exhaust valve significantly impacts both the performance and durability of an engine. This study presents a data-driven approach to optimizing exhaust valve geometry, focusing on reducing wear loss and enhancing sealing effectiveness between the valve and seat ring in a diesel engine under thermal and structural analysis. Utilizing a design of experiments (DOE) approach, the study considers six geometric parameters of the valve and a friction coefficient to evaluate their effects on wear loss and sealing performance. The friction coefficient was identified as the most critical factor for wear loss, while the contact angle and length were key in influencing sealing between the components.

Two machine learning models using random forest were developed to predict sealing effectiveness and wear volume loss. These models were then used in an optimization procedure employing a Multi-objective Genetic Algorithm (MOGA). The optimal design was selected through multi-criteria decision-making methods (MCDM), Technique for Order of Preference by Similarity to Ideal Solution (TOPSIS), and VIKOR. The optimized model selected by TOPSIS outperformed the initial model by improving the contact ratio by 24% and reducing wear loss by 58% compared to the initial model. This study demonstrates the potential for significant advancements in exhaust valve design through data-driven optimization, leading to improved performance and efficiency in diesel engines.

# Empowering organizations with Engineering Intelligence to revolutionize product development

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## 1 Summary

In this talk, we will demonstrate how the Neural Concept (NC) platform enables engineers to develop end-to-end AI-enhanced workflows, driven by historical data from simulations, completely integrated into their current workflows and with online simulation capabilities. The combination of predictive and generative AI models empowers engineers to efficiently evaluate a significantly larger number of designs than with traditional simulation tools and reach optimized results with better performance much faster.

We will focus our attention on selected use cases to demonstrate this end-to-end integration of NC within comprehensive engineering workflows for complex designs. Currently, NC is being used by multiple organizations in workflows including, but not limited to, the following applications: heat exchanger design optimization, structural analysis and durability studies, internal flows, external aerodynamics for air and road vehicles, turbomachinery, electronics testing, and e-motor optimization.

## 2 Introduction and context

In today's highly competitive landscape, engineering organizations face increasing pressure to deliver complex, high-performing products at an accelerated pace, all while managing tighter margins. To maintain an edge, teams must shorten design cycles and enhance product performance and quality simultaneously.

However, traditional simulation and optimization tools often fall short of meeting the demands of today's fast-moving production environments. Design teams struggle to fully utilize the insights from these tools and seamlessly integrate them into their workflows. Engineering Intelligence (EI) represents a significant advancement, leveraging modern AI techniques to overcome these challenges.

### 2.1 Engineering Intelligence

Engineering Intelligence (EI) combines technology, engineering expertise, and advanced software tools like CAE, CAD, and PLM to accelerate product development from the initial concept to market launch. It is born from AI techniques, but adapted to the specific needs of the engineering field.

At the heart of EI is "quantitative AI," which merges human-like intelligence (such as LLMs, generative AI, etc.) with the quantitative intelligence that is the core of our technology (such as surrogate models). LLMs are not enough in the precise world of engineering; that's where the quantitative layer steps in. EI is the next step in AI's journey, evolving and adapting to meet the constraints of engineering work.

EI is changing the game for engineers. It's not just about improving current ways of working; it's about moving towards fully independent design processes. However, EI isn't just a set of tools; it's a field in its own right, with experts, specific tools, and its own platform.

EI unlocks a new era in product design. Its sophisticated generative design capabilities, coupled with more dynamic automation options, enable designers to leverage past data to dramatically speed up simulations.

Embracing EI transforms the way products come to life, integrating simulation, CAD, and engineering data into a smart, unified platform that accelerates the product development lifecycle from concept to market. By drawing on enterprise engineering knowledge and established methodologies, EI facilitates near-autonomous design, significantly reducing development time.

## 2.2 CAE Data Scientists

CAE Data Scientists are at the heart of the EI transformation, blending their deep knowledge of computer-aided engineering (CAE) with data science. These professionals are key players in advancing the creation of products, making the process more efficient and pushing performance to new heights, quickly and proficiently.

In the fast-moving world of product development, these engineers excel in applying advanced AI methodologies and are proficient with fundamental data science tools such as Python. As part of an elite group within their field, CAE Data Scientists lead the charge in transforming traditional design workflows into AI-driven processes. They hold a unique combination of technical knowledge, practical skills, and a keen willingness to innovate and tackle the complex challenges they encounter.

## 2.3 Neural Concept Platform

The Neural Concept (NC) platform offers a seamless way for engineers to incorporate AI-driven workflows into their existing practices. It utilizes past simulation data to create a fully integrated system with real-time simulation capabilities. By harnessing the power of both predictive and generative AI models, the platform allows engineers to quickly and efficiently explore a significantly larger set of design alternatives compared to conventional simulation tools and to achieve optimal results with enhanced performance in a shorter time frame.

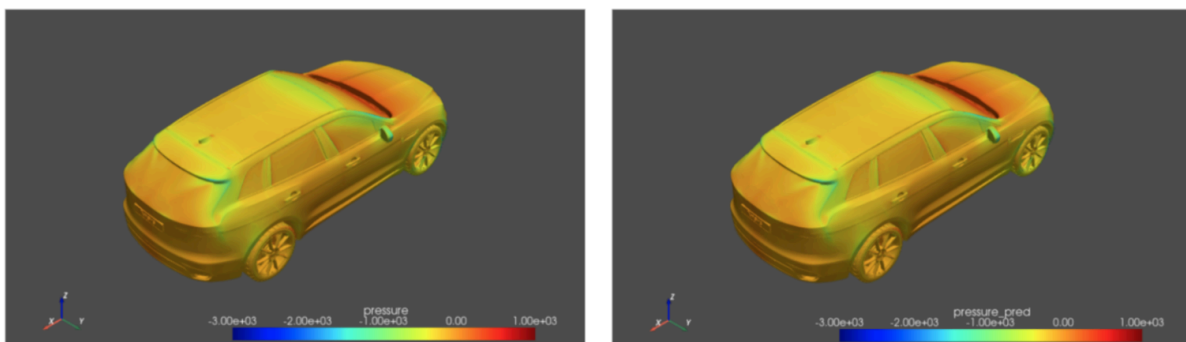
Our innovative platform is designed to create impact across three integrated layers:

- **Core:** which uses advanced AI and deep learning to turn underutilized CAE/CAD data into actionable insights.
- **Studio:** which overcomes traditional infrastructure constraints by embedding engineering data and optimization into interactive tools.
- **Platform:** which supports the deployment, sharing, and maintenance of EI-powered workflows.

## 3 EI workflow examples for specific applications

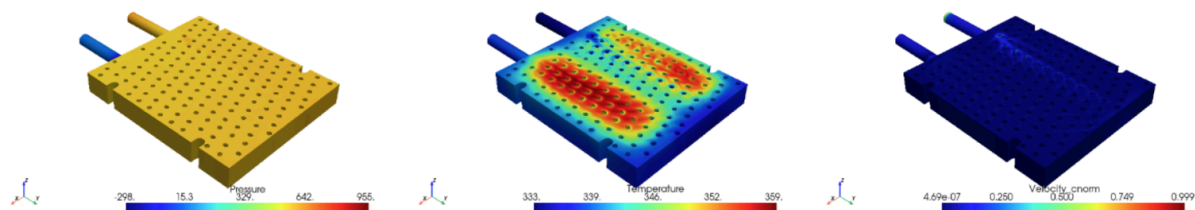
In this talk, we will explore the development of NC-integrated workflows for several different applications, focusing on end-to-end workflows for selected use cases, such as vehicle external aerodynamics, heat exchanger optimization, and e-motor optimization.

In vehicle external aerodynamics, the main motivation for designers is to improve performance and reduce aerodynamic drag and the corresponding fuel consumption and emissions. Evaluating multiple design variations with traditional simulation tools is extremely expensive as design iterations increase. NC enables engineers and designers to iterate fast and explore the design space efficiently, at a massively reduced computational cost and achieving improved design performance. Central to this approach is the generative design capability of the platform to explore variations of baseline designs quickly, combined with state-of-the-art predictive algorithms.



**Fig. 1.** Comparison of pressure field prediction on the surface of an SUV between CFD results (ground truth, left) and prediction using an NC predictive model (right).

In the application of heat exchanger design, engineers need to optimize between the competing objectives of reducing the pressure loss through the heat exchanger and ensuring the maximum heat transfer to minimize the peak temperature while maintaining uniformity to some extent. Similarly, the increasing cost of simulating multiple designs and the restricted capabilities of design generation using parametric geometry generation tools prevent engineers and designers from reaching true optimal designs within their design space. NC combines flexible, non-parametric generative models to explore new geometries with accurate predictive models to evaluate their performance, allowing designers to explore the design space efficiently and achieve improved designs while massively reducing the design cycle time.



**Fig. 2.** Heat exchanger design. Visualization of the pressure drop (left), the temperature distribution (center), and the velocity (right) for a generated heat exchanger geometry.

Beyond aerodynamics and heat exchanger applications, we will also briefly review other related uses of NC for applications within structural mechanics, electric motor design, battery thermal management, and others.

## 4 Conclusions

The current landscape of engineering is compelling designers and engineers to work together more closely than ever, with the aim to enhance product performance dramatically within significantly reduced design cycles.

By leveraging the latest advancements in predictive and generative AI tools, Neural Concept is enabling engineers to develop optimized products much more rapidly compared to traditional methods. Numerous companies and organizations globally are turning to the NC platform to fold their established workflows into AI-augmented, data-oriented processes, capitalizing on both historical design data and in-house expertise, along with the most recent developments in Deep Learning.

In this new era of Engineering Intelligence it's essential for engineers to adapt and use the latest technology in order to develop products with superior performance at a previously unattainable speed.

